NEUTRONS AND THEIR INTERACTION WITH MATTER

Auteur - Date

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NEUTRONS FOR SOCIETY

NEUTRONS AND THEIR INTERACTION WITH MATTER

Overview

- *History – neutrons and nuclear reactions*
- *Production – reactors and spallation sources*
- *Properties – as a particle and a probe*
- Instruments – exploiting the probe to do science

A BIT OF HISTORY

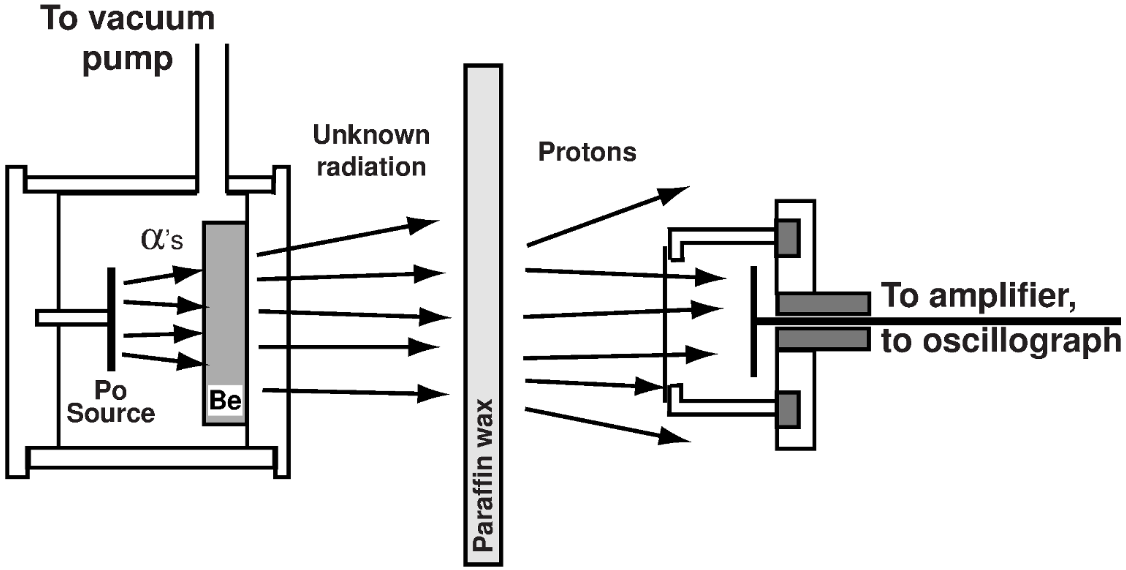
The neutron

- 1932: J. Chadwick, after work by others, discovers the 'neutron', a neutral but massive particle

$$ {}^{4}_{2}\mathrm{He} + {}^{9}_{4}\mathrm{Be} \rightarrow {}^{12}_{6}\mathrm{C} + {}^{1}_{0}\mathrm{n} $$

$$ \left(m_{He} + m_{B}\right)c^{2} + T_{He} = \left(m_{C} + m_{n}\right)c^{2} + T_{C} + T_{n} $$

$$ m_{n} = 1.0067 \pm 0.0012 \text{ a.m.u} $$



A BIT OF HISTORY

The nuclear reaction

- 1938: O. Hahn, F. Strassmann & L. Meitner discovered the fission of ^{235}U nuclei through thermal neutron capture
- 1939: H. v. Halban, F. Joliot & L. Kowarski showed that ^{235}U nuclei fission produced 2.4 neutrons on average – chain reaction
- 1942: E. Fermi & al. demonstrated first self-sustained chain reaction reactor

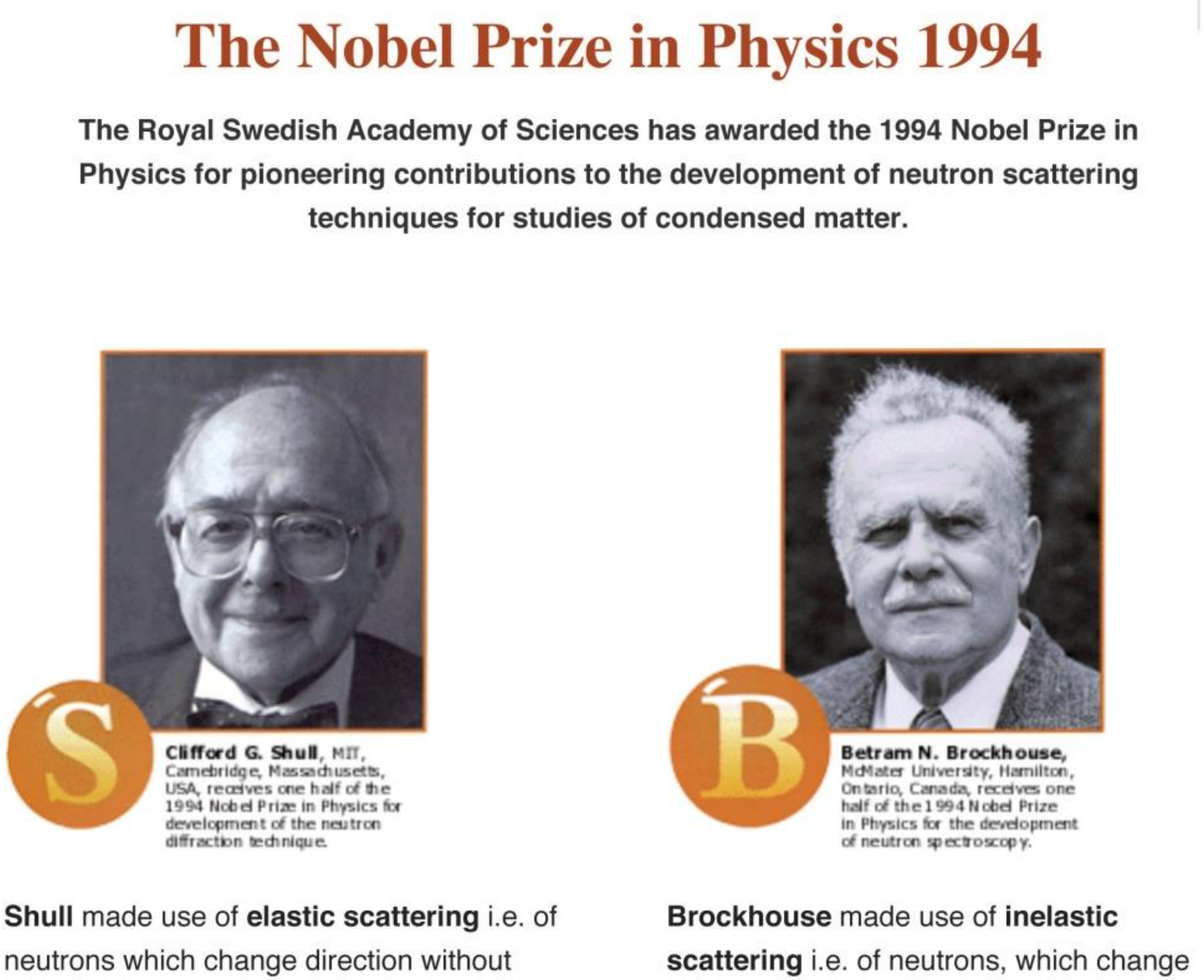
Chicago pile:
360T of graphite
50T of U and UO
0.5W power


OPPENHEIMER
HISTORY VS. HOLLYWOOD

NOBEL PRIZES, NEUTRONS AND THE ILL

Chadwick, Shull & Brockhouse

James Chadwick
(1891 - 1974)



The Nobel Prize in Physics 1994

The Royal Swedish Academy of Sciences has awarded the 1994 Nobel Prize in Physics for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter.

Clifford G. Shull, MIT, Camebridge, Massachusetts, USA, receives one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.

Betram N. Brockhouse, McMater University, Hamilton, Ontario, Canada, receives one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.

Shull made use of **elastic scattering** i.e. of neutrons which change direction without

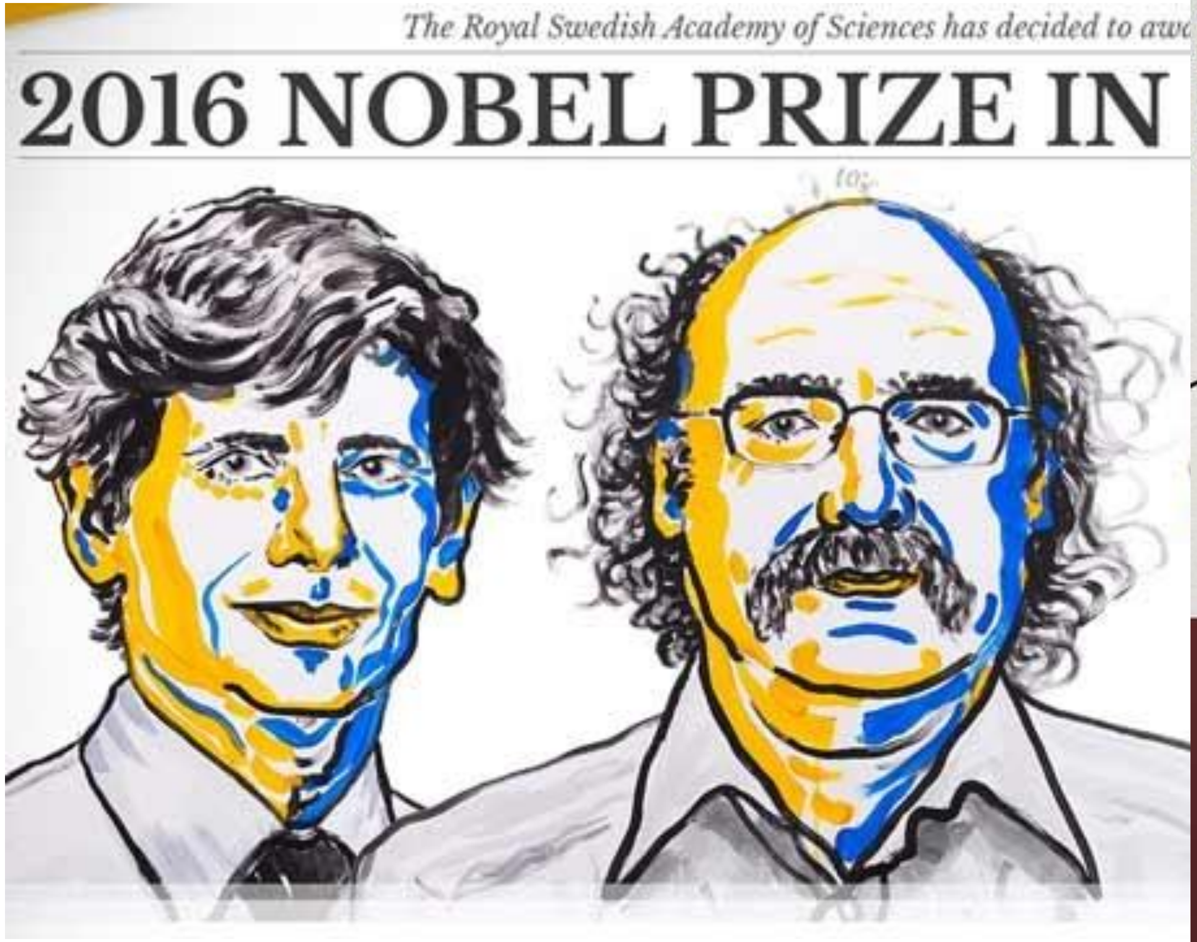
Brockhouse made use of **inelastic scattering** i.e. of neutrons, which change

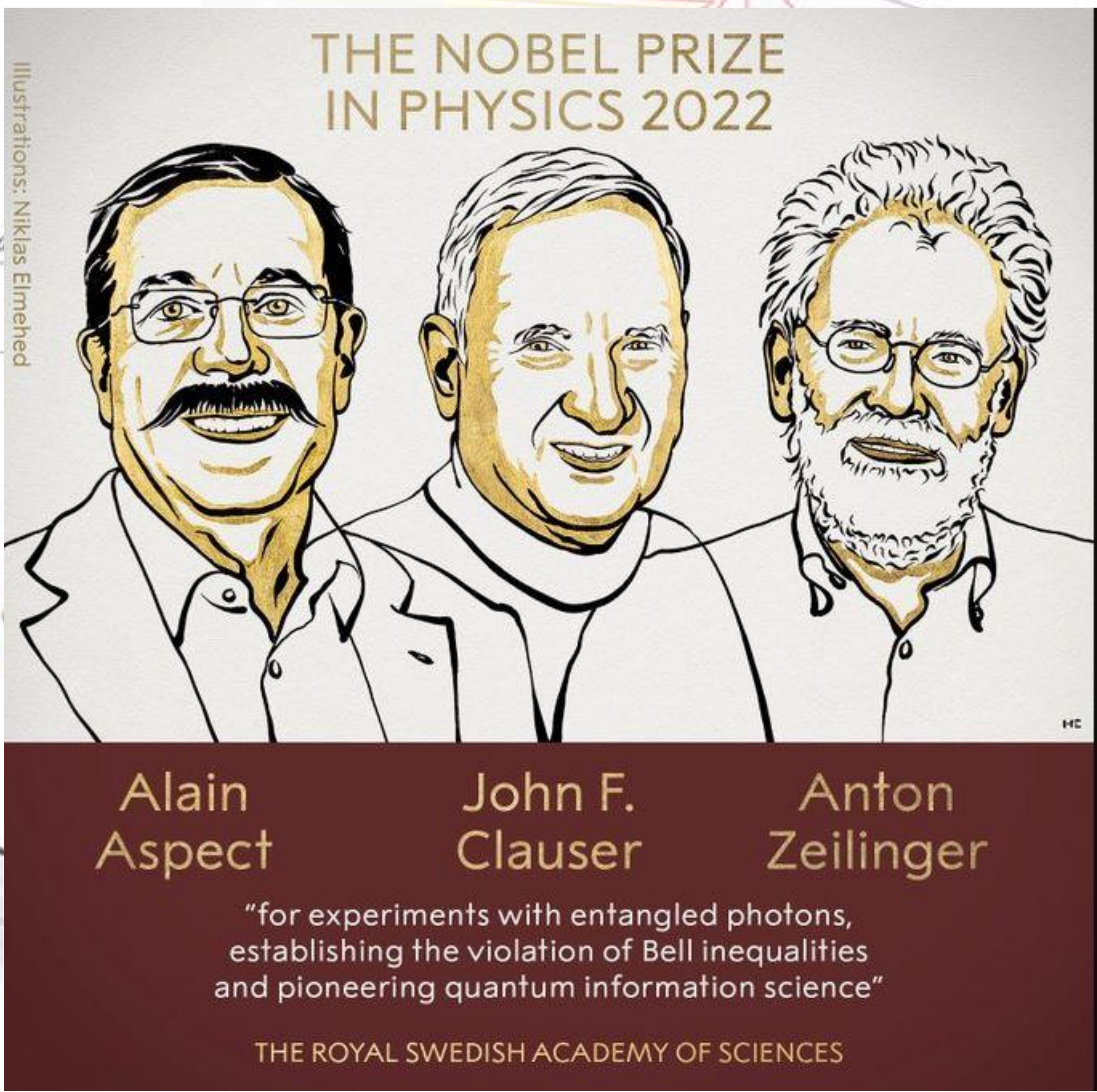
NOBEL PRIZES, NEUTRONS AND THE ILL

Louis Néel
(Grenoble) -
magnetism

NOBEL PRIZES, NEUTRONS AND THE ILL

Haldane (1977 – 1981), Kosterlitz and Thouless for topological phase transitions and phases of matter (Electronic structure and excitation of 1D quantum liquids and spin chains)



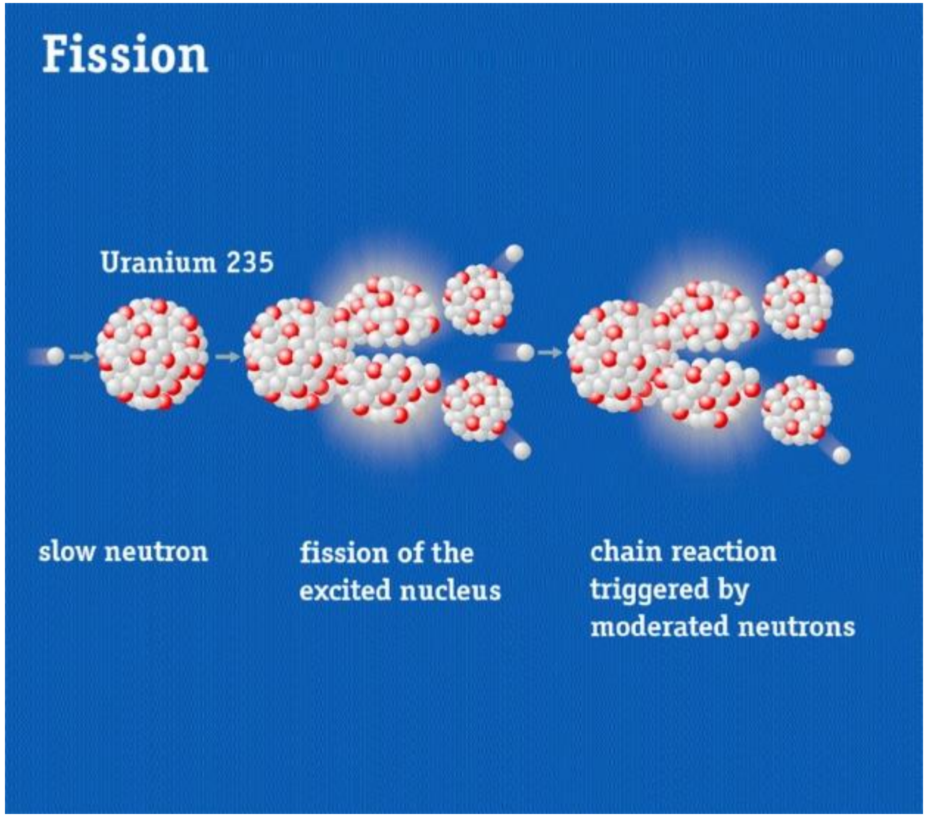


"for experiments with entangled photons, establishing the violation of Bell inequalities and pioneering quantum information science"

NEUTRON SOURCES

Fission reactors

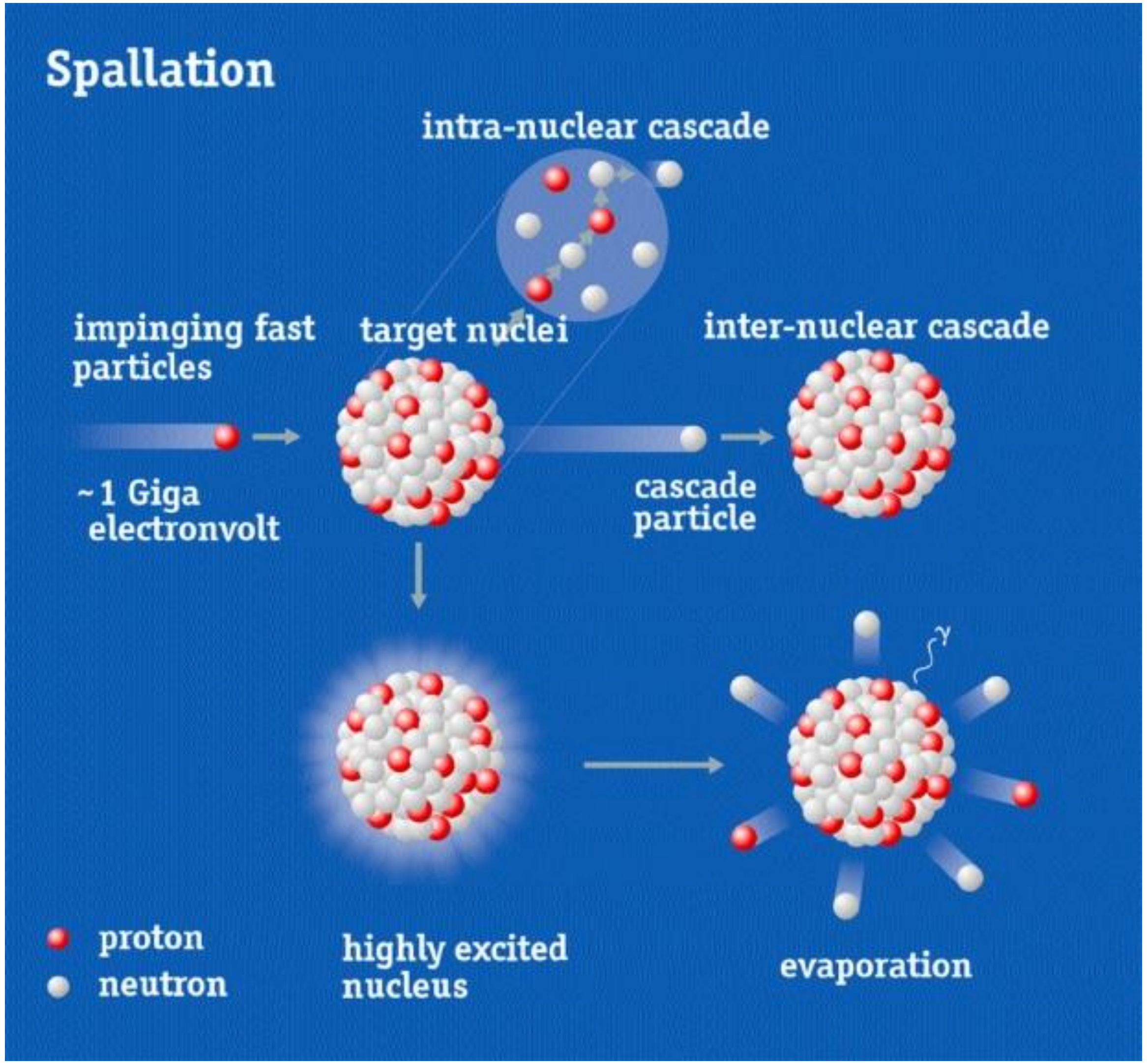
- Nuclear fission → chain reaction with excess neutrons (1n → 2.5n)
- Slow neutrons split U-235 nuclei
- Fission neutrons have MeV energies and need to be moderated (thermalized) to meV energies by scattering from water
- Thermalisation @ RT → *thermal* neutrons, @ 25K → *cold* neutrons and @ 2400 K → *hot* neutrons
- ILL – flux 1.5 x 10^{15} n/cm^2/s



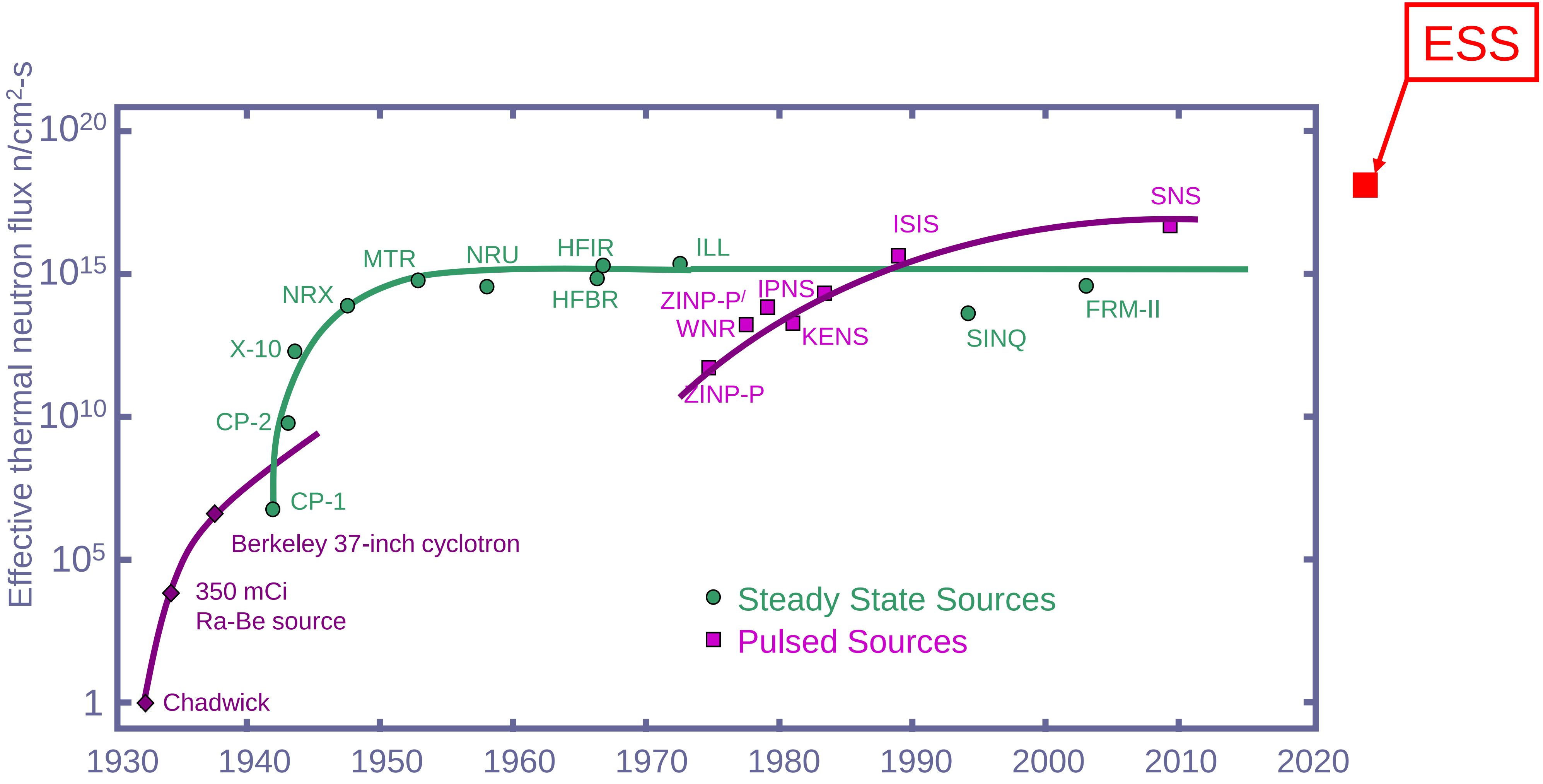
NEUTRON SOURCES

Spallation sources

- Neutrons can be produced by bombarding heavy metal targets
- 2 GeV protons (90% speed-of-light) produce spallation – evaporation of ~30 neutrons



Neutron sources



(Updated from *Neutron Scattering*, K. Skold and D. L. Price, eds., Academic Press, 1986)

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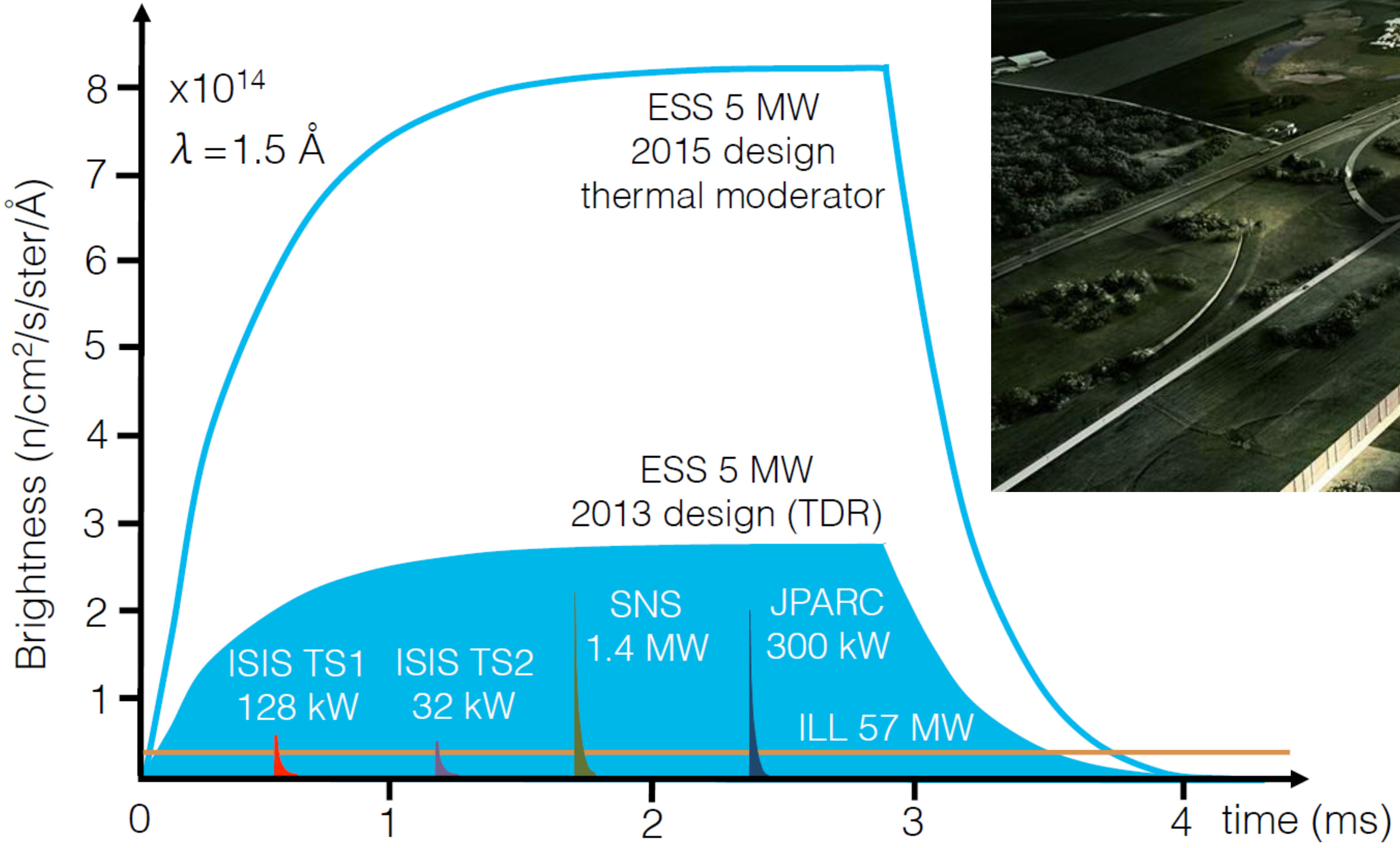
CONTINUOUS OR PULSED BEAMS

Integrated vs peak flux – ESS will have a time-integrated flux comparable to ILL



CONTINUOUS OR PULSED BEAMS

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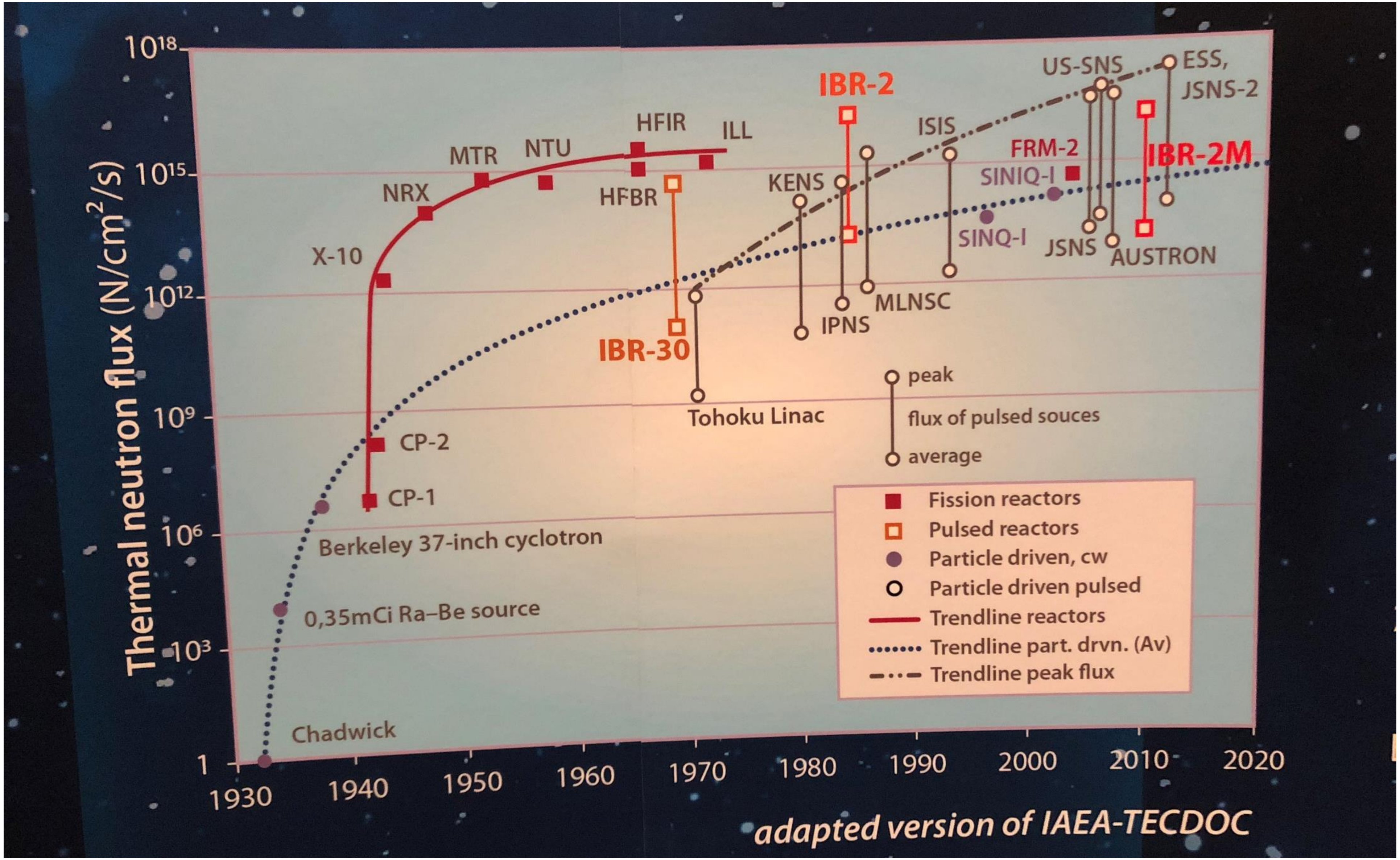
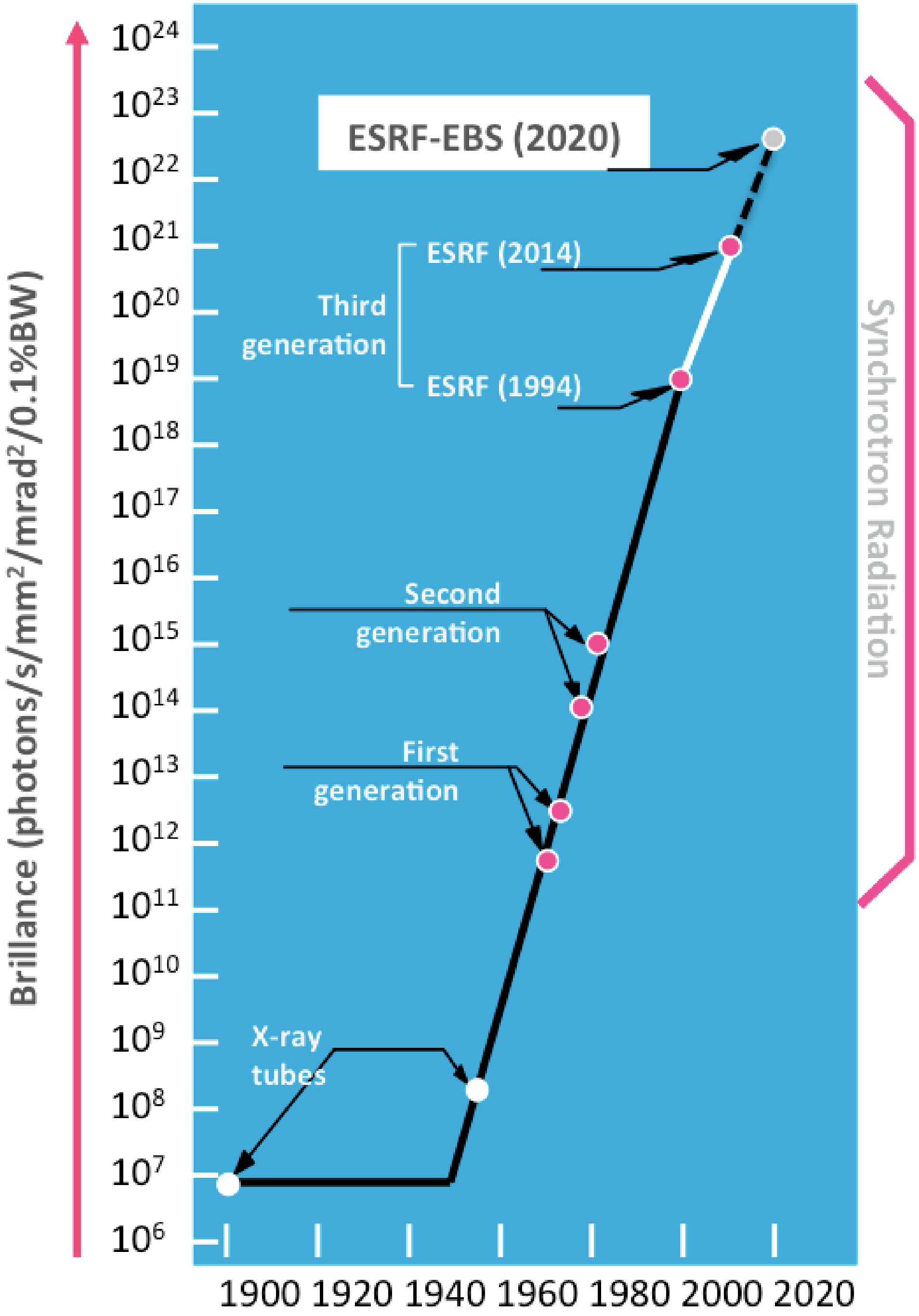


adapted version of IAEA-TECDOC

N vs X

ESRF (hard X-rays)

- Exponential development contrasts with development of neutron sources



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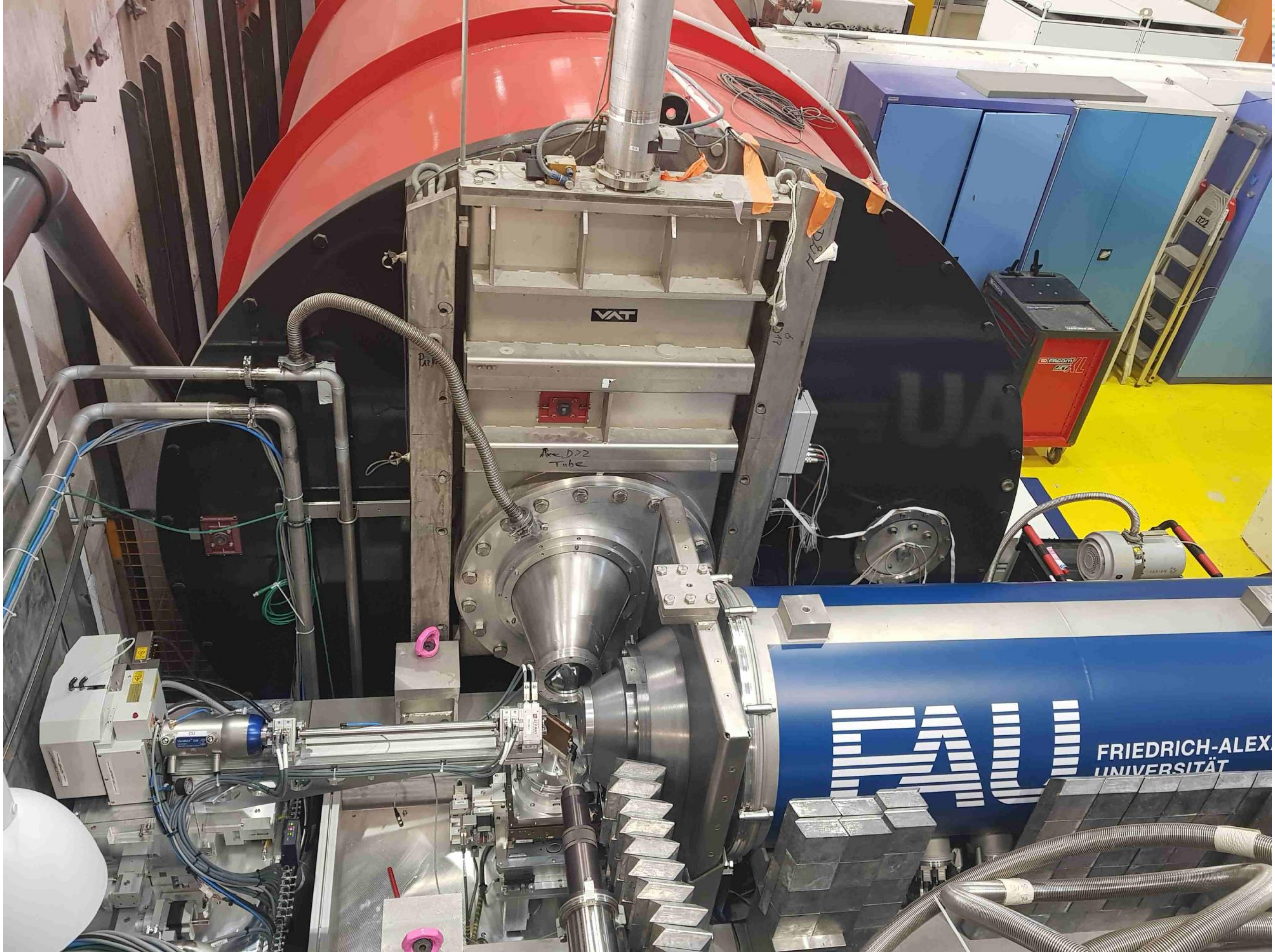
N & X



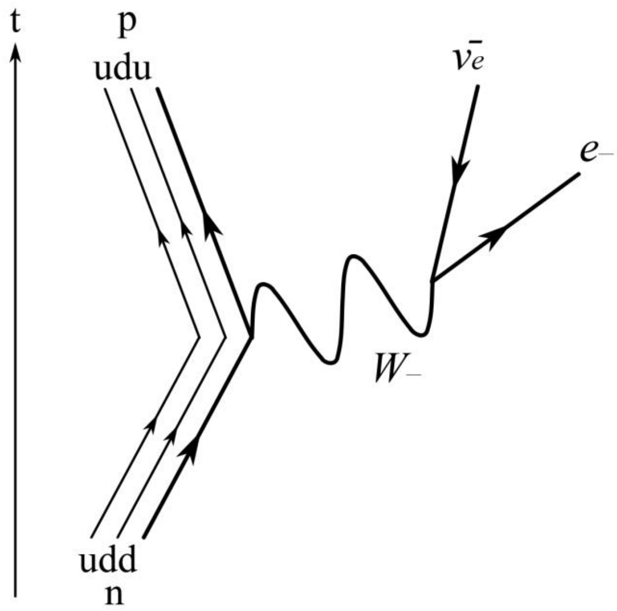
THE NEUTRON

As a particle

- free neutrons are unstable: β-decay → proton, electron, anti-neutrino

  life time: 888 ± 1 sec or 880 ± 1 sec

- wave-particle duality: neutrons have particle-like and wave-like properties
- mass: $m_n = 1.675 \times 10^{-27}$ kg = 1.00866 amu. (unified atomic mass unit)
- charge = 0
- spin =1/2
- magnetic dipole moment: $\mu_n = -1.9\ \mu_N$, $\mu_p = 2.8\ \mu_N$, $\mu_e \sim 10^3\ \mu_n$,
- velocity (v), kinetic energy (E), temperature (T), wavevector (k), wavelength (λ)



THE NEUTRON

As a particle

- velocity (v), kinetic energy (E), temperature (T), wavevector (k), wavelength (λ)

$$E = m_n v^2/2 = k_B T = (hk/2\pi)^2/2m_n = (h/\lambda)^2/2m_n$$

- Neutron energy determines velocity and therefore time-of-flight (*tof*) over a given distance i.e. *tof* → energy determination

$$tof = \frac{L}{v} = 253\mu\sec\cdot\lambda\left[\overset{o}{A}\right]\cdot L[m]$$

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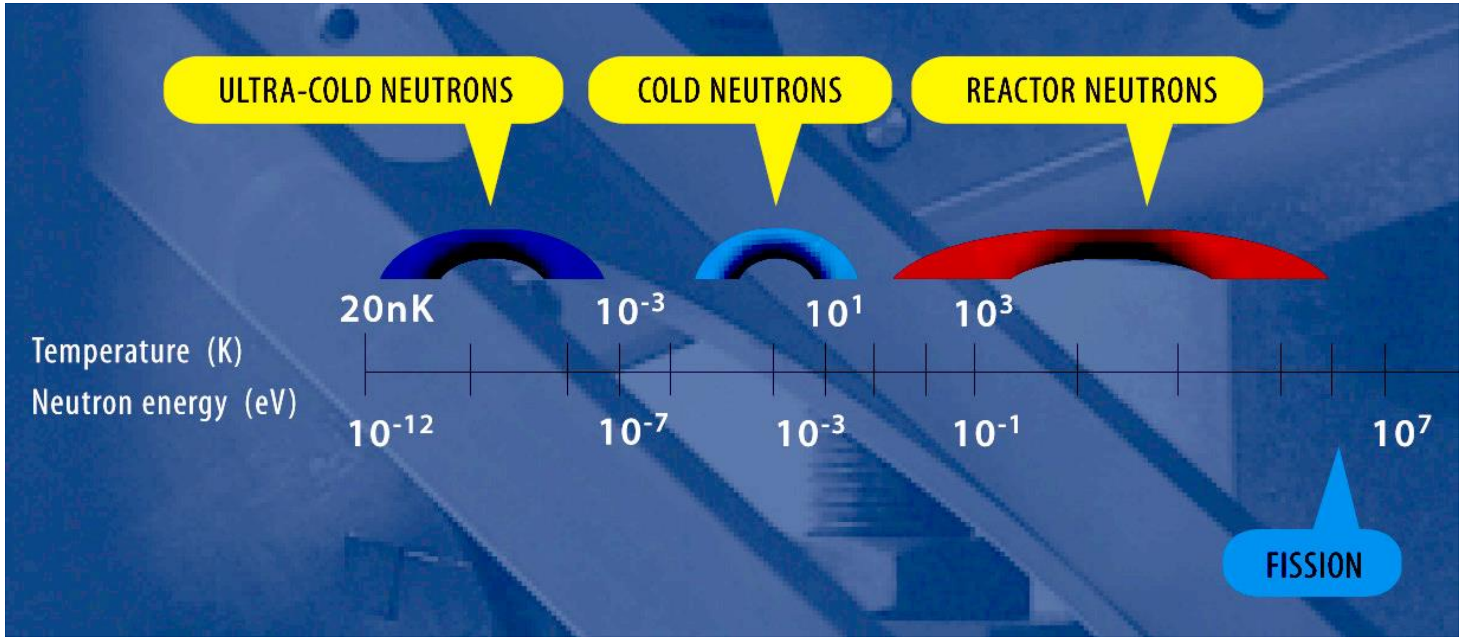
THE NEUTRON

As a probe

	Energy	Temperature (K)	Wavelength (nm)	velocity (m/s)
Ultra cold neutrons	< 10 µeV	< 0.05	> 30	< 15
Cold neutrons	100 - 5000 µeV	1 - 60	0.4 - 3	150 - 1000
Thermal neutrons	5 - 50 meV	60 - 600	0.13 - 0.4	1000 - 4000
Hot neutrons	0.05 - 0.5 eV	600 - 6000	0.04 - 0.13	4000 - 10000



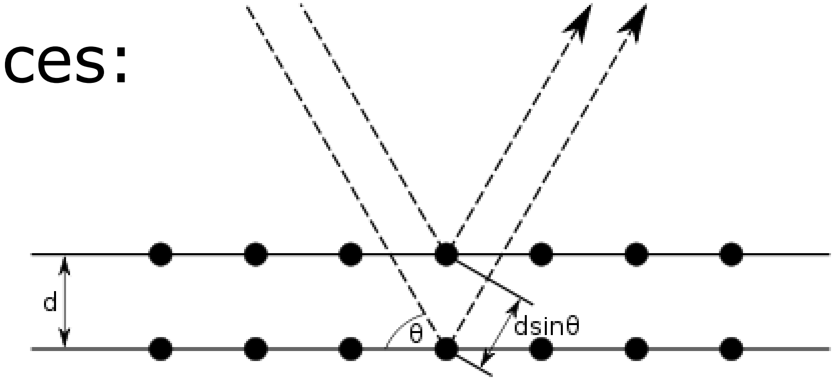

adixen

THE NEUTRON

As a probe

- Wavelengths on the scale of inter-atomic distances: *Å - nm* wavelengths to measure *Å - μm* distances/sizes

$$n\lambda = 2d\sin\Theta$$



- Energies comparable to structural and magnetic excitations: *meV* neutrons to measure *neV – meV* energies
- Neutral particle – gentle probe, highly penetrating (e.g. 30 cm of Al), no radiation damage (low flux & energy)
- Magnetic moment (nuclear spin) probes magnetism of unpaired electrons (N.B. $\mu_e \sim 1000\text{x}\ \mu_N$)

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THE NEUTRON

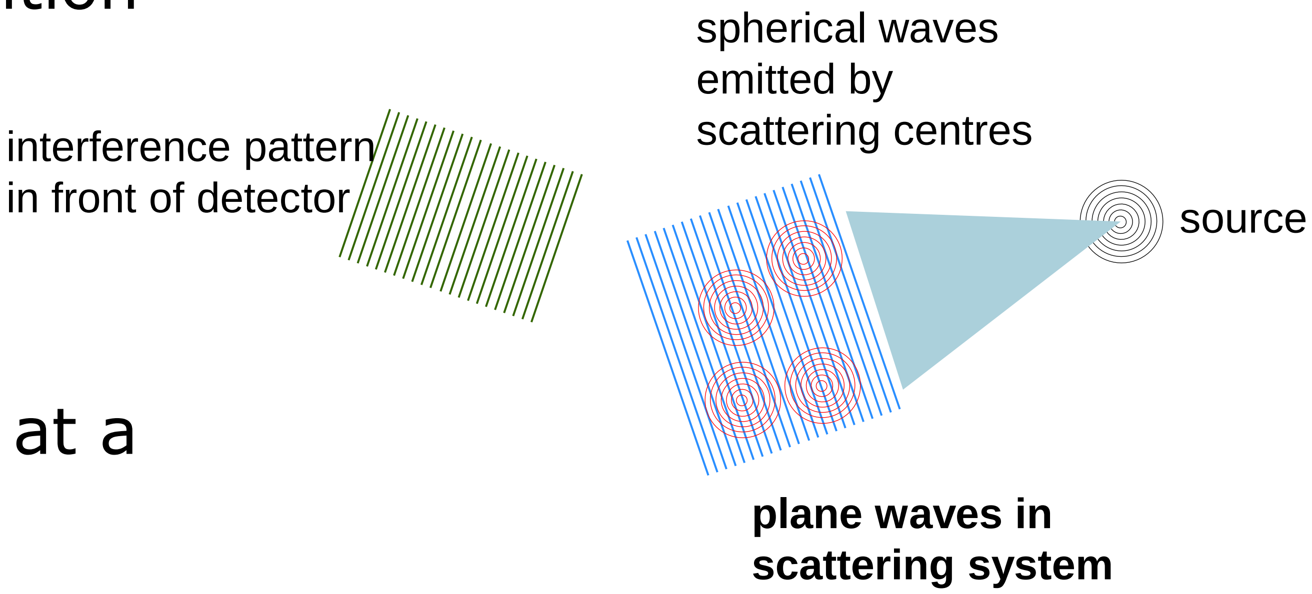
As a probe – interacting with matter – scattering from atoms

- Neutron flux at reactor core
- 1.5×10^{15} n/cm^2/s
- Flux at an instrument sample position
- 10^8 n/cm^2/s

→ 10^{-6} n/μm^2/μs

→ 10^{-15} n/nm^2/ns

- On these time and length scales, neutrons are being scattered one at a time
- Need wave-particle duality of neutrons



THE NEUTRON

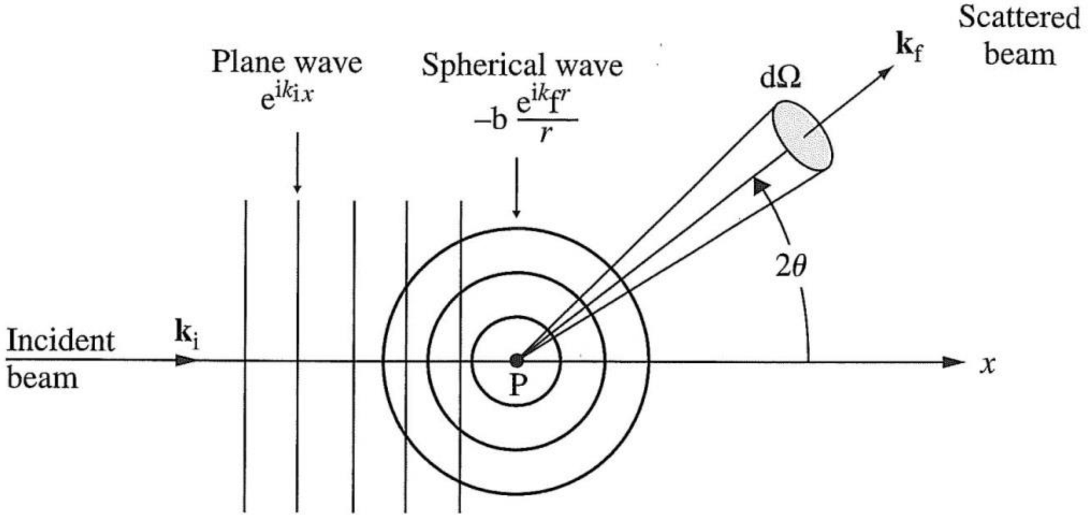
As a probe – interacting with matter – (elastic) scattering from a single fixed nucleus

$$- b \frac{e^{i\mathbf{k}_f . \mathbf{r}}}{r}$$

- Nuclear size << neutron wavelength → point-like s-wave scattering
- b is the scattering length (‘power’) in *fm*
- #neutrons scattered per second per unit solid angle Ω: $\Psi^2 r^2 d\Omega$

$$d\sigma/d\Omega = b^2$$

- σ is the cross-section: $4\pi b^2$ (in barns – 100 fm^2)



$$V(\mathbf{r}) = \frac{2p\hbar^2}{m_r} b\, d(\mathbf{r})$$

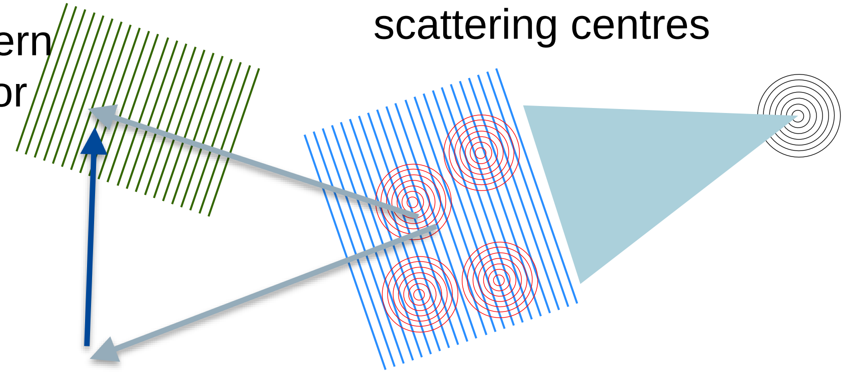
THE NEUTRON

As a probe – interacting with matter – scattering from a set of nuclei

$$\frac{d\sigma}{d\Omega} = \sum_{j,k} b_j b_k e^{i\vec{Q}.\left(\vec{R}_j - \vec{R}_k\right)}$$

$$\vec{Q} = \vec{k}_f - \vec{k}_i$$

- Q is called momentum transfer
- Q-dependence (e.g. angle) gives info about atomic positions



THE NEUTRON

As a probe – interacting with matter – scattering from a set of identical nuclei – coherent and incoherent scattering

- Set of *N* similar atoms/ions – spins/isotopes are *uncorrelated* at different sites
- *b* depends on spin/isotope
- Average is ‹*b*›
- Incoherent scattering gives a *Q* independent background
- But it can be useful to probe the dynamics of single particles (later)

$$\frac{d\sigma}{d\Omega} = \langle b\rangle^2 \sum_{j,k} e^{iQ\cdot(R_j - R_k)} + \left(\langle b^2\rangle - \langle b\rangle^2\right) N$$

$$\sigma_{coh} = 4\pi\langle b\rangle^2 \qquad \sigma_{coh} = 4\pi b_{coh}{}^2$$

$$\sigma_{incoh} = 4\pi\left(\langle b^2\rangle - \langle b\rangle^2\right) \qquad \sigma_{incoh} = 4\pi b_{inc}{}^2$$

NEUTRONS FOR SOCIETY

THE NEUTRON

As a probe – interacting with matter – scattering from a set of identical nuclei – coherent and incoherent scattering

- If single isotope and zero nuclear spin, no incoherent scattering
- If single isotope and non-zero nuclear spin I
- nucleus+neutron spin: $I+1/2$ and $I-1/2$ scattering length b^+ and b^-
- To reduce incoherent scattering (background):
  - polarise nuclei and neutrons
  - use isotope substitution e.g. H→ D

$$\langle b \rangle = \frac{1}{2I+1}\left[(I+1)b^{+} + Ib^{-}\right]$$

$$\langle b^2 \rangle - \langle b \rangle^2 = \frac{I(I+1)}{(2I+1)^2}\left(b^{+} - b^{-}\right)^2$$

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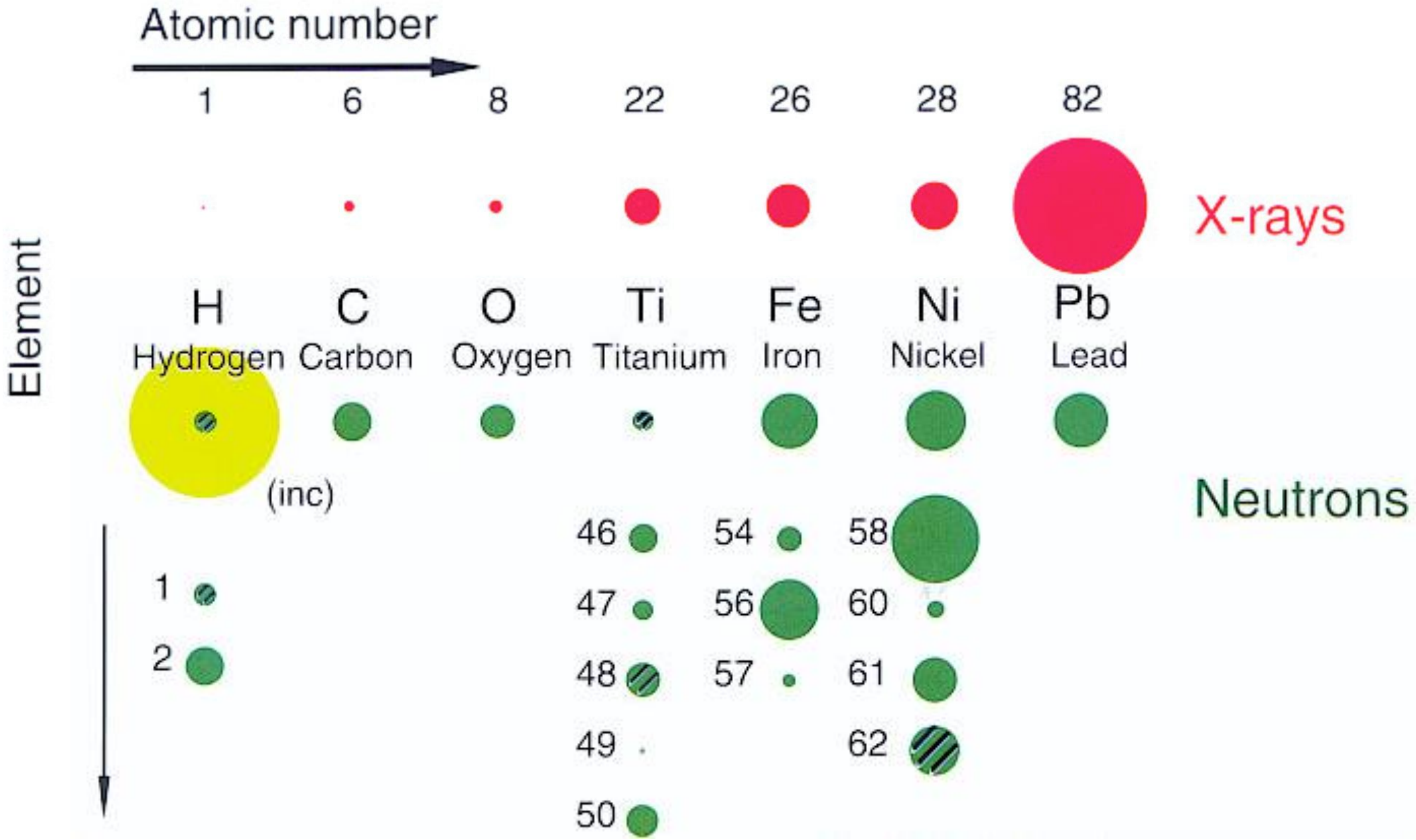
THE NEUTRON

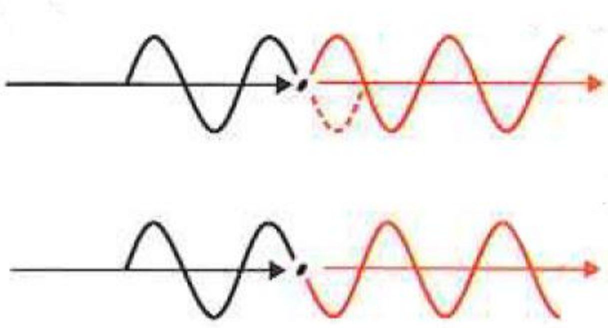
Scattering lengths
Light atoms
Contrast

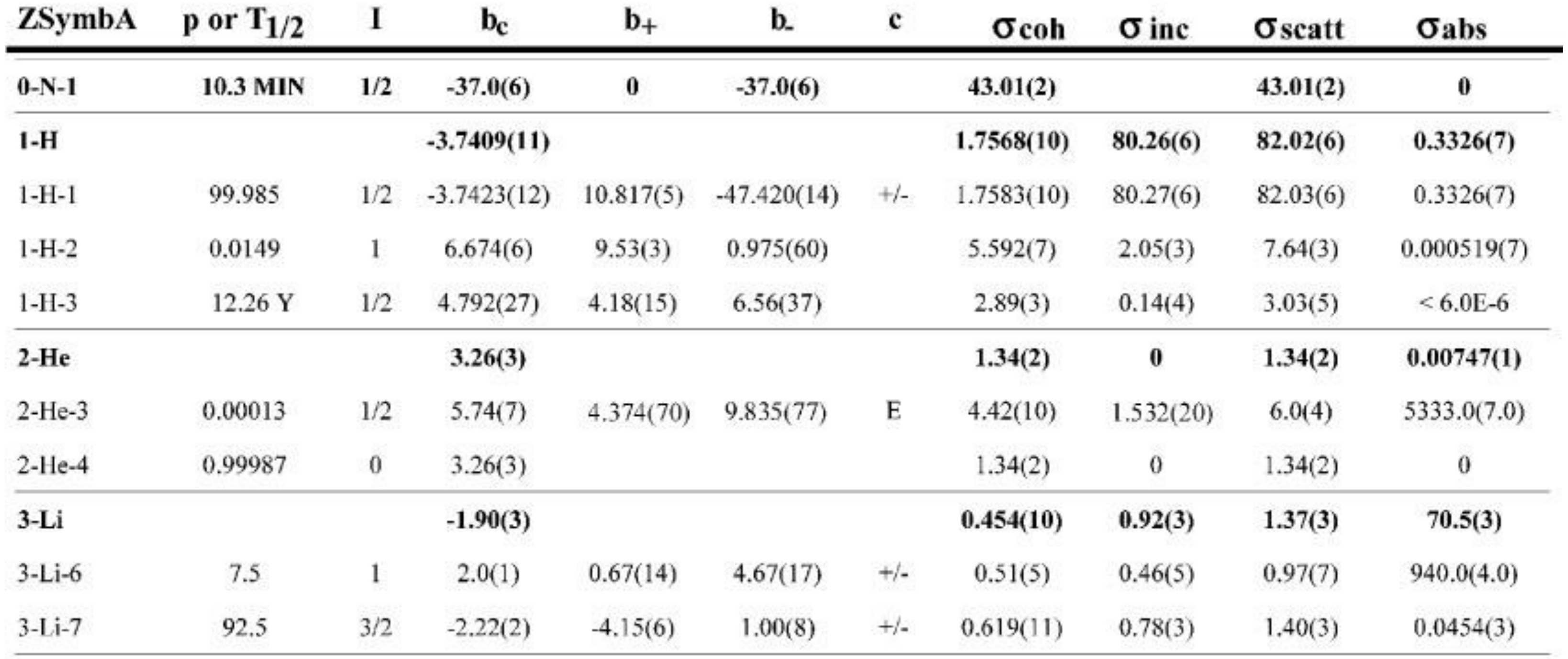


THE NEUTRON

Scattering lengths can be positive or negative (nuclear physics)

- Positive *b* (most nuclei): phase change
- Negative *b*: no phase change at scattering point

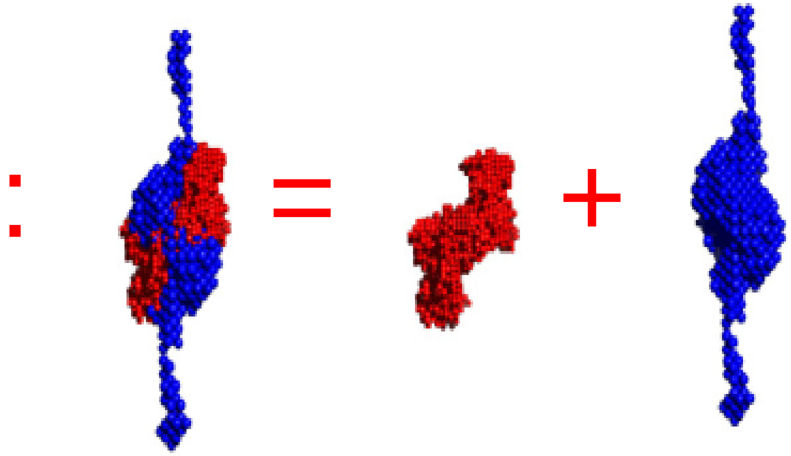


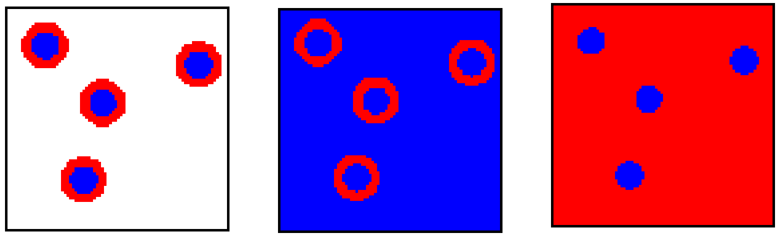


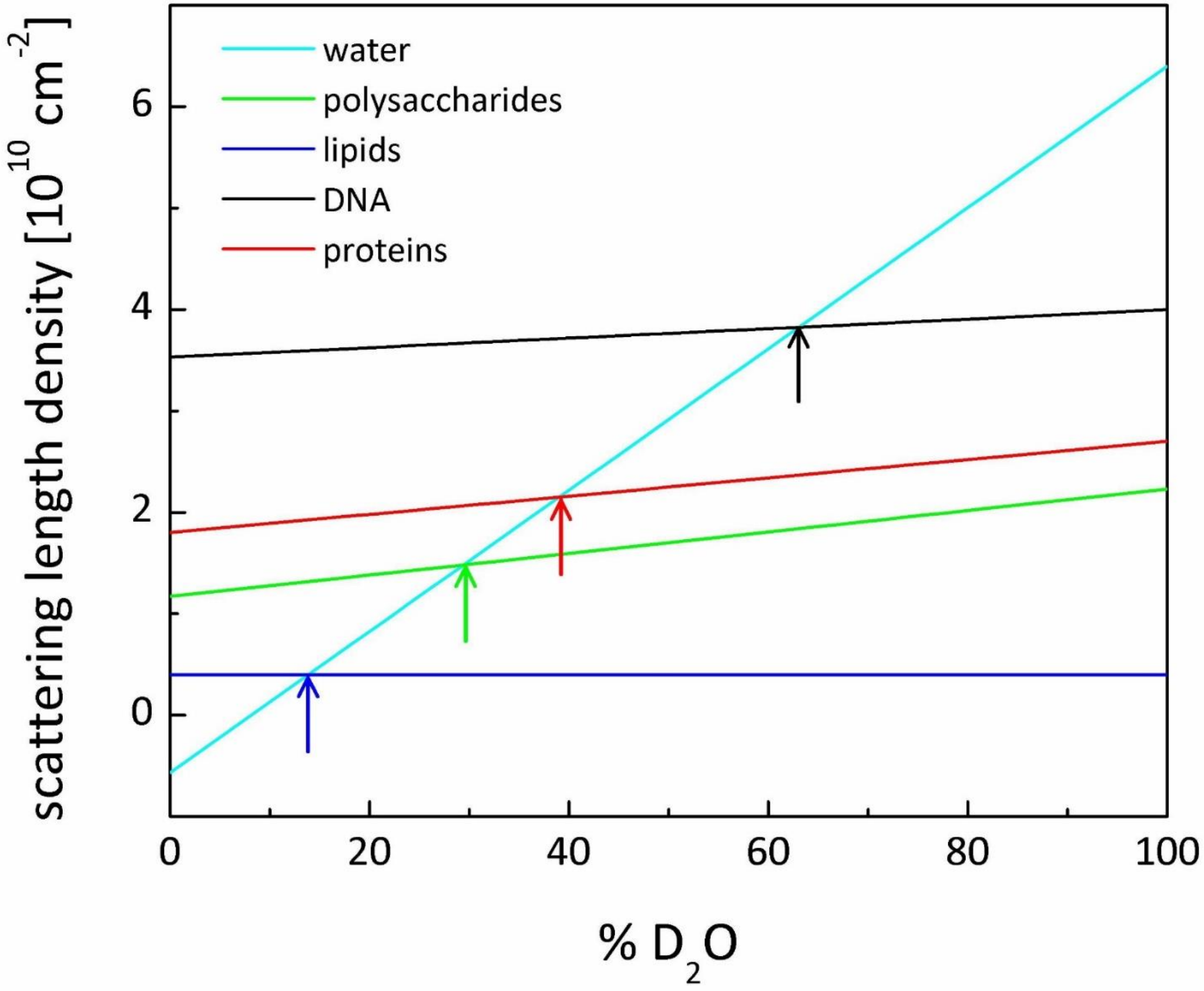
ZSymbA	p or $T_{1/2}$	I	b_c	b_+	b_-	c	σ_{coh}	σ_{inc}	σ_{scatt}	σ_{abs}
0-N-1	**10.3 MIN**	**1/2**	**-37.0(6)**	**0**	**-37.0(6)**		**43.01(2)**		**43.01(2)**	**0**
1-H			**-3.7409(11)**				**1.7568(10)**	**80.26(6)**	**82.02(6)**	**0.3326(7)**
1-H-1	99.985	1/2	-3.7423(12)	10.817(5)	-47.420(14)	+/-	1.7583(10)	80.27(6)	82.03(6)	0.3326(7)
1-H-2	0.0149	1	6.674(6)	9.53(3)	0.975(60)		5.592(7)	2.05(3)	7.64(3)	0.000519(7)
1-H-3	12.26 Y	1/2	4.792(27)	4.18(15)	6.56(37)		2.89(3)	0.14(4)	3.03(5)	< 6.0E-6
2-He			**3.26(3)**				**1.34(2)**	**0**	**1.34(2)**	**0.00747(1)**
2-He-3	0.00013	1/2	5.74(7)	4.374(70)	9.835(77)	E	4.42(10)	1.532(20)	6.0(4)	5333.0(7.0)
2-He-4	0.99987	0	3.26(3)				1.34(2)	0	1.34(2)	0
3-Li			**-1.90(3)**				**0.454(10)**	**0.92(3)**	**1.37(3)**	**70.5(3)**
3-Li-6	7.5	1	2.0(1)	0.67(14)	4.67(17)	+/-	0.51(5)	0.46(5)	0.97(7)	940.0(4.0)
3-Li-7	92.5	3/2	-2.22(2)	-4.15(6)	1.00(8)	+/-	0.619(11)	0.78(3)	1.40(3)	0.0454(3)

THE NEUTRON

Scattering lengths can be positive or negative
→ Contrast matching





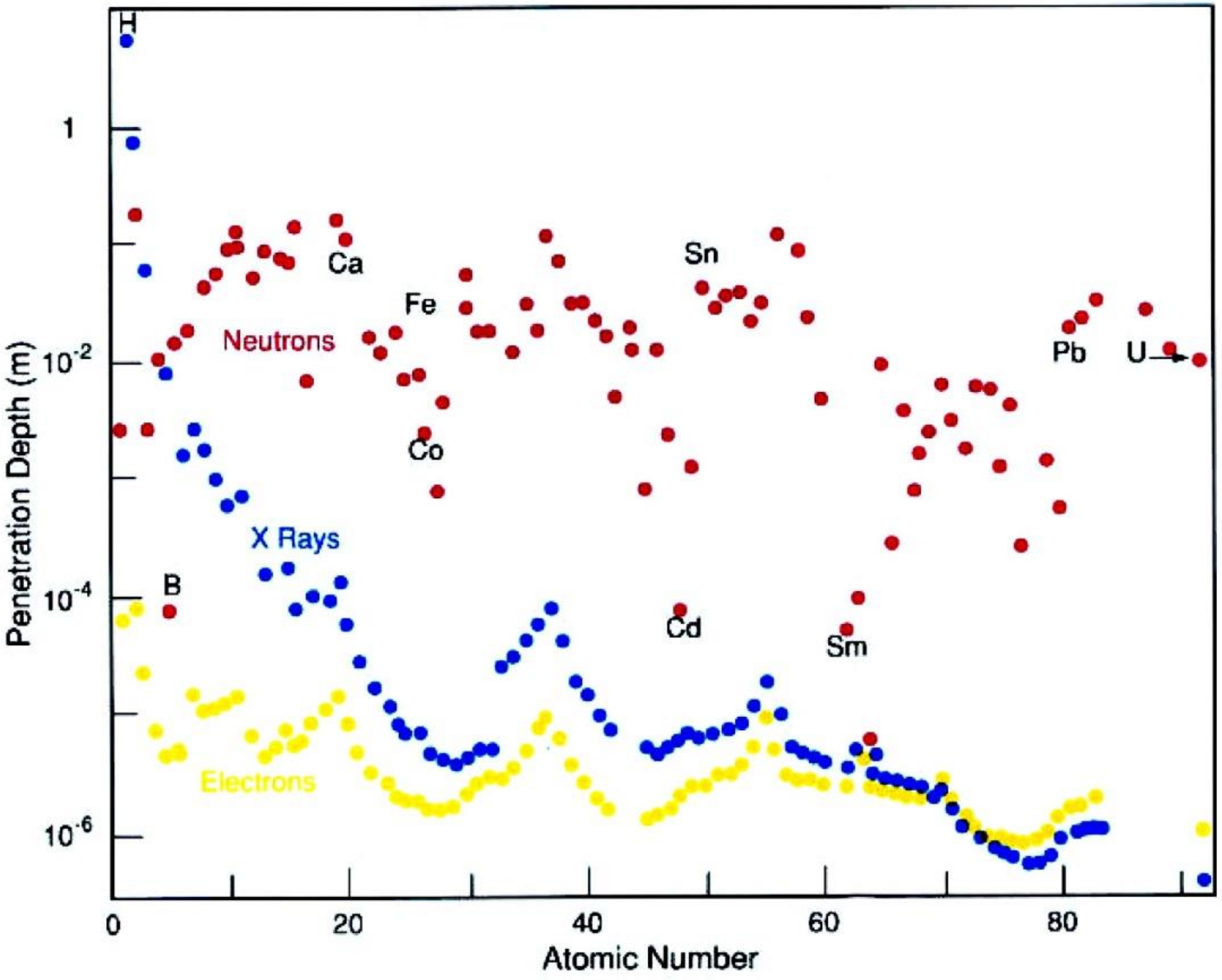


THE NEUTRON

As a probe – interacting with matter - absorption

- Absorption – neutron capture
- Several strong absorbers:

  He, Li, B, Cd, Gd,…
- Isotope dependent – choose to your advantage



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THE NEUTRON

As a probe – interacting with matter - absorption - Neutron detection

- How to detect a weakly interacting, neutral particle?
- With a neutron absorber and measure the resulting signal

$$^{3}_{2}\mathrm{He} + {}^{1}_{0}\mathrm{n} \rightarrow {}^{3}_{1}\mathrm{H} + \mathrm{p} + 0.764\ \mathrm{MeV}$$

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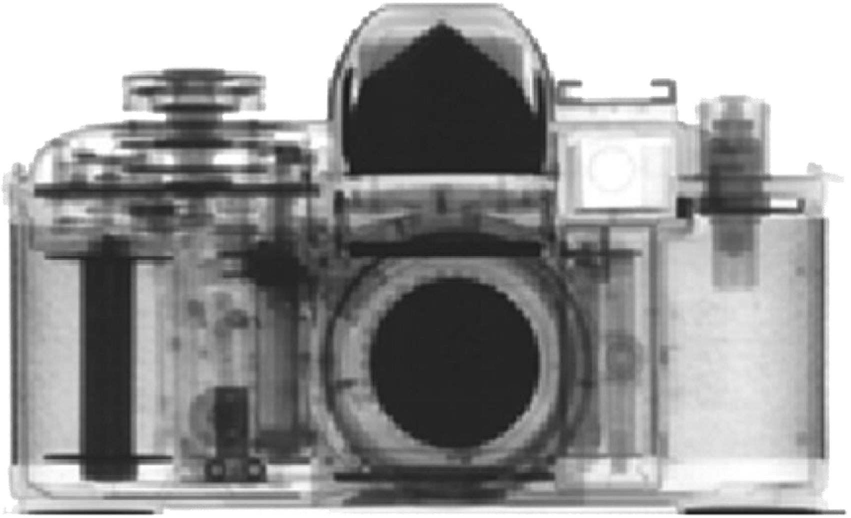
THE NEUTRON

Scattering and absorption cause attenuation of a neutron beam → imaging

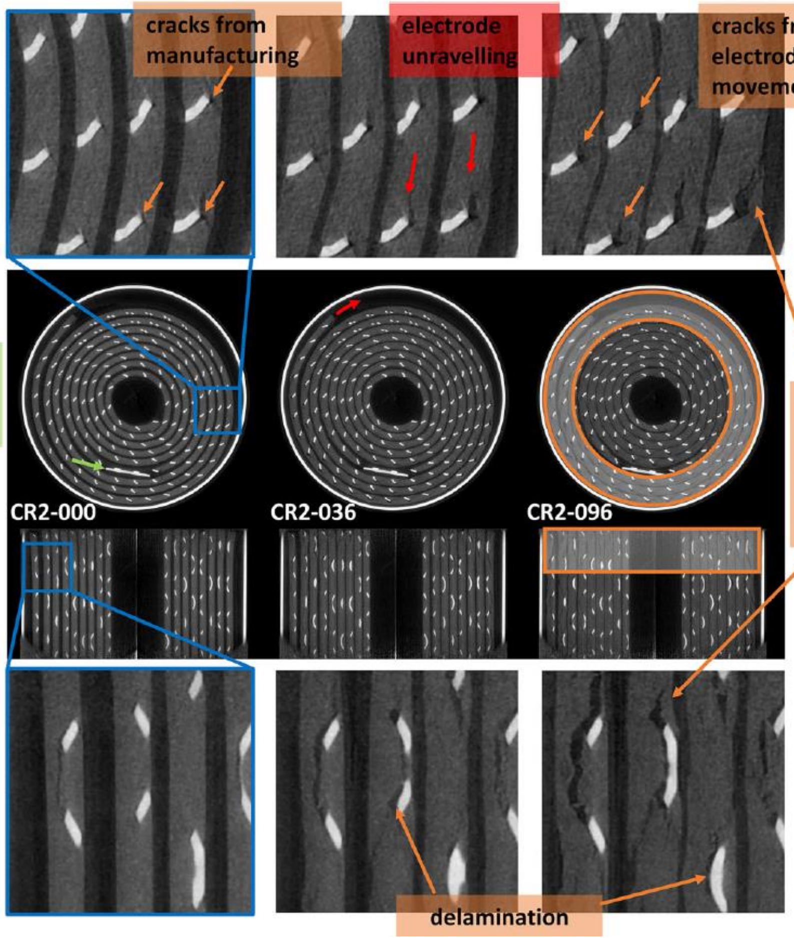


NEUTRONS

X-RAYS

THE NEUTRON

Imaging Li-ion batteries - NATURE COMM | https://doi.org/10.1038/s41467-019-13943-3



cracks from manufacturing

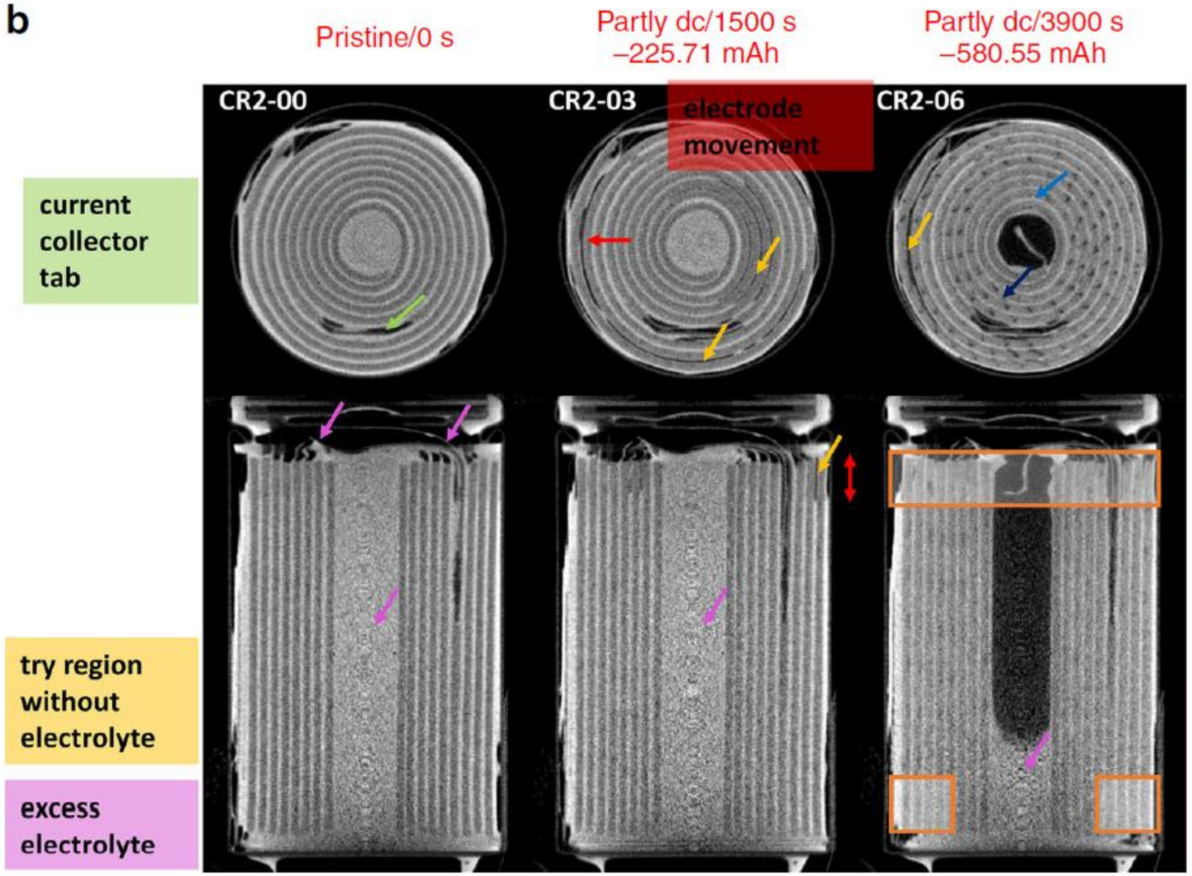
electrode unravelling

cracks from electrode movement

current collector tab

regions of strong electrode cracking

delamination



electrode movement

current collector tab

try region without electrolyte

excess electrolyte

less lithium removal

higher lithium removal

2 mm of strong lithiation during first dc period

regions of strong electrode cracking

THE NEUTRON

As a probe – interacting with matter - summary

- Interaction with nuclei:
  - short range interaction → angle independent scattering (no form factor)
  - scattering length can be positive or negative (→ contrast variation)
  - depends on isotope (→ selectivity) and nuclear spin
  - Coherent and incoherent scattering – strength and weakness
  - Scattering contrast different from X-rays, favours light atoms
- A gentle probe – low intensity, meV neutron beam does not cause radiation damage like a ~10 keV photon beam (what about XFEL!)
- Magnetic moment probes magnetism of unpaired electrons

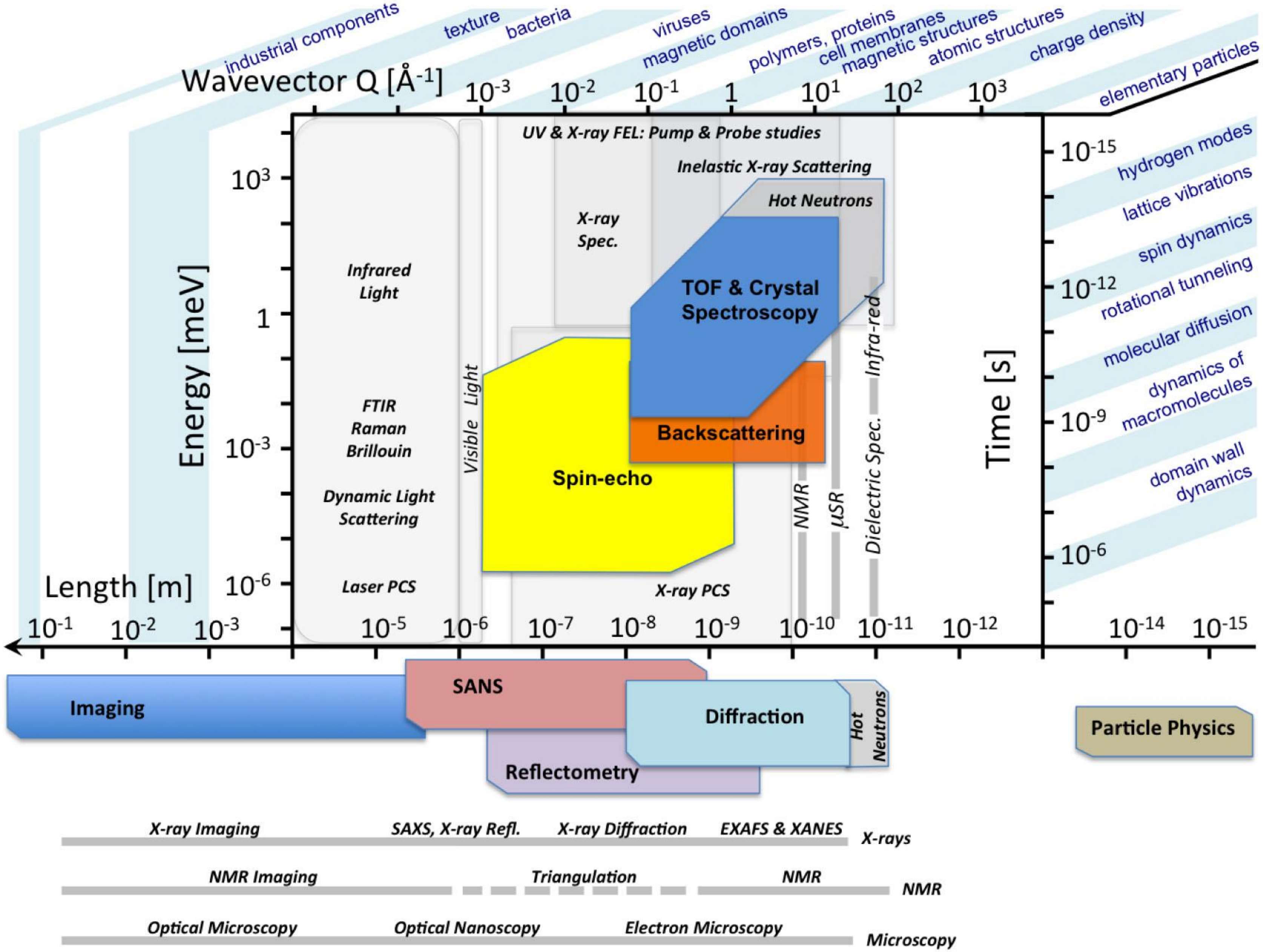
NEUTRONS AND THEIR INTERACTION WITH MATTER

Overview

- History – neutrons and nuclear reactions
- Production – reactors and spallation sources
- Properties – as a particle and a probe
- *Instruments – exploiting the probe to do science*

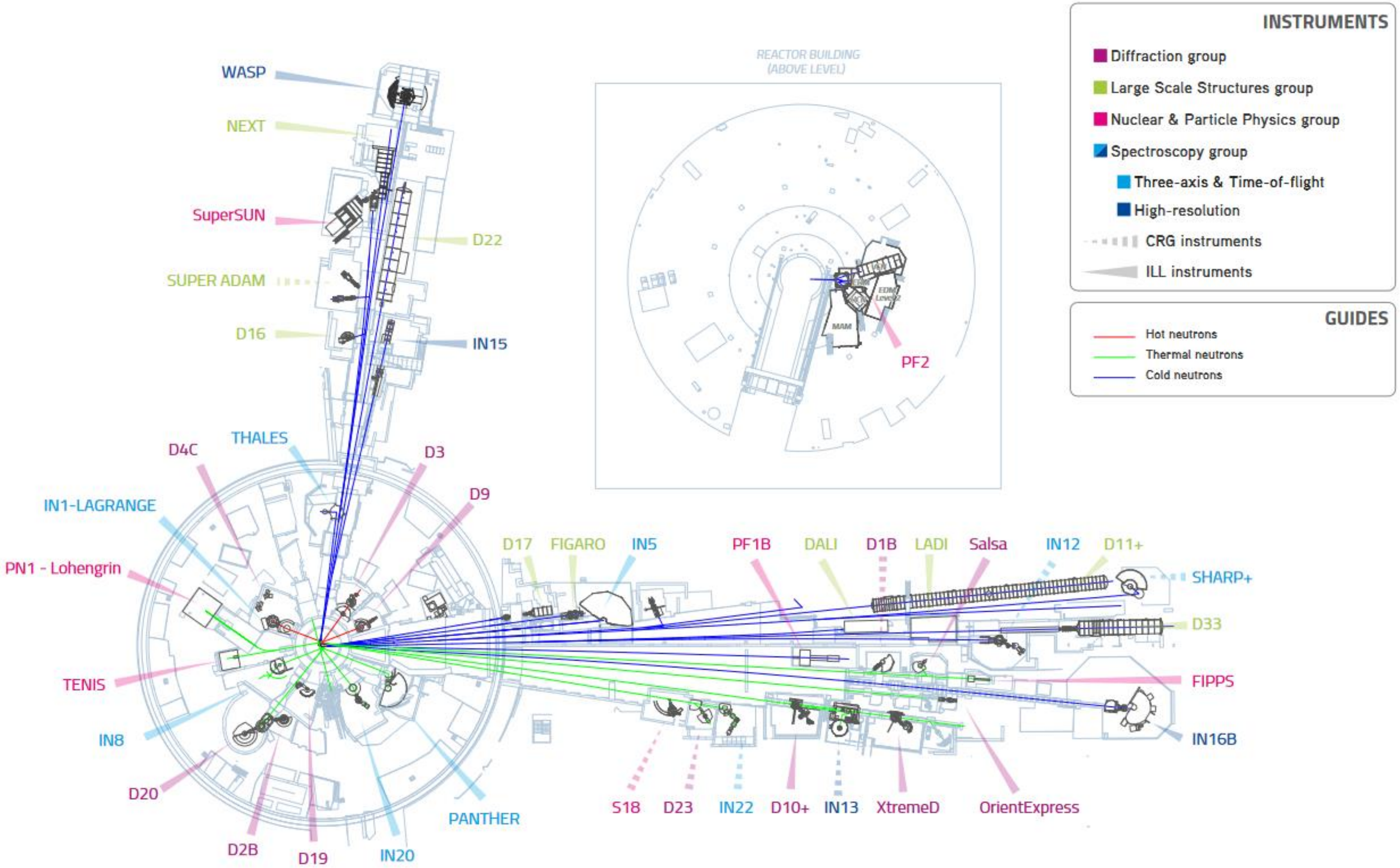
INSTRUMENTS & SCIENCE

Time
and
length
scales



NEUTRONS FOR SOCIETY

THE ILL’S INSTRUMENT SUITE



GENERAL EXPRESSION FOR SCATTERING FROM A COMPLEX SYSTEM

Deriving the general scattering function

Based on

- Born approximation – kinematic theory: neutron wavefunction un-perturbed inside sample
- Fermi's Golden Rule to calculate transitions of neutron (k) and system (λ) from initial and final state
- Hamiltonian to describe the system states (λ)

$$\frac{d\sigma}{d\Omega} = \frac{\sum\limits_{k_f \, in \, d\Omega} W_{k_i,\lambda_i \to k_f,\lambda_f}}{\Phi \; d\Omega}$$

$$\sum_{k_f \, in \, d\Omega} W_{k_i,\lambda_i \to k_f,\lambda_f} = \frac{2\pi}{\hbar} \rho_{\mathbf{k}_f} \left| \langle \mathbf{k}_f \lambda_f | V | \mathbf{k}_i \lambda_i \rangle \right|^2$$

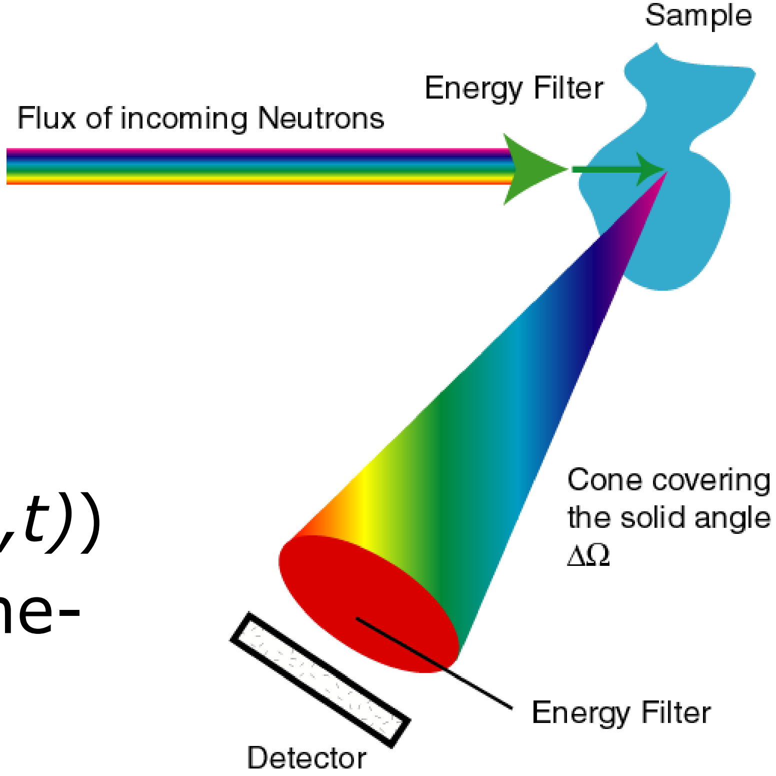
$$\left(\frac{d^2\sigma}{dE_f \, d\Omega} \right)_{\lambda_i \to \lambda_f} = \frac{k_f}{k_i} \left(\frac{m_n}{2\pi\hbar^2} \right)^2 \left| \langle \mathbf{k}_f \lambda_f | V | \mathbf{k}_i \lambda_i \rangle \right|^2 \delta\left(E_i - E_f + E_{\lambda_i} - E_{\lambda_f} \right)$$

GENERAL EXPRESSIONS FOR SCATTERING FROM A SET OF MOVING ATOMS

Deriving the scattering function – end up with (after much algebra and manipulations!)

$$\left(\frac{d^2\sigma}{dEd\Omega}\right)=\frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{jk}b_jb_k\int_{-\infty}^{+\infty}\left\langle \exp\left\{-i\vec{Q}\cdot\vec{R}_j(0)\right\}\exp\left\{i\vec{Q}\cdot\vec{R}_k(t)\right\}\right\rangle\exp(i\omega t)dt$$

$$\left(\frac{d^2\sigma}{dEd\Omega}\right)=\frac{k_f}{k_i}\frac{1}{2\pi\hbar}S(\vec{Q},\omega)$$



- Experiment measures double differential cross-section which is simply related to *S(Q,ω)* (or *I(Q,t)*)
- *S(Q,ω)* is the double Fourier transform of the time-dependent pair-correlation function

NEUTRONS FOR SOCIETY

GENERAL EXPRESSIONS FOR SCATTERING FROM A SET OF MOVING ATOMS

Deriving the scattering function – end up with coherent & incoherent contributions

- For a simple system with a single element but different *b*’s

$$\left.\frac{d^2\sigma}{d\Omega dE_f}\right)_{coh} = \frac{\sigma_{coh}}{4\pi}\frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{jk}\int_{-\infty}^{+\infty}\left\langle \exp\left\{-i\vec{Q}\cdot\vec{R}_j(0)\right\}\exp\left\{i\vec{Q}\cdot\vec{R}_k(t)\right\}\right\rangle \exp(-i\omega t)\,dt$$

$$\left.\frac{d^2\sigma}{d\Omega dE_f}\right)_{incoh} = \frac{\sigma_{incoh}}{4\pi}\frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{j}\int_{-\infty}^{+\infty}\left\langle \exp\left\{-i\vec{Q}\cdot\vec{R}_j(0)\right\}\exp\left\{i\vec{Q}\cdot\vec{R}_j(t)\right\}\right\rangle \exp(-i\omega t)\,dt$$

- Scattering function determined by positions *R* of different atoms at different times *t*
- Incoherent scattering can be useful: it measures the correlation between the same atom at different times → single particle dynamics - diffusion

GENERAL SCATTERING EXPERIMENT

Scattering triangle – handling Q and ω

- $\boldsymbol{Q=k_f - k_i}$, $\hbar\omega=E_f - E_i$ $(E \sim k^2,\ k = 2\pi/\lambda)$

- Elastic scattering:

  vary Q without changing ω

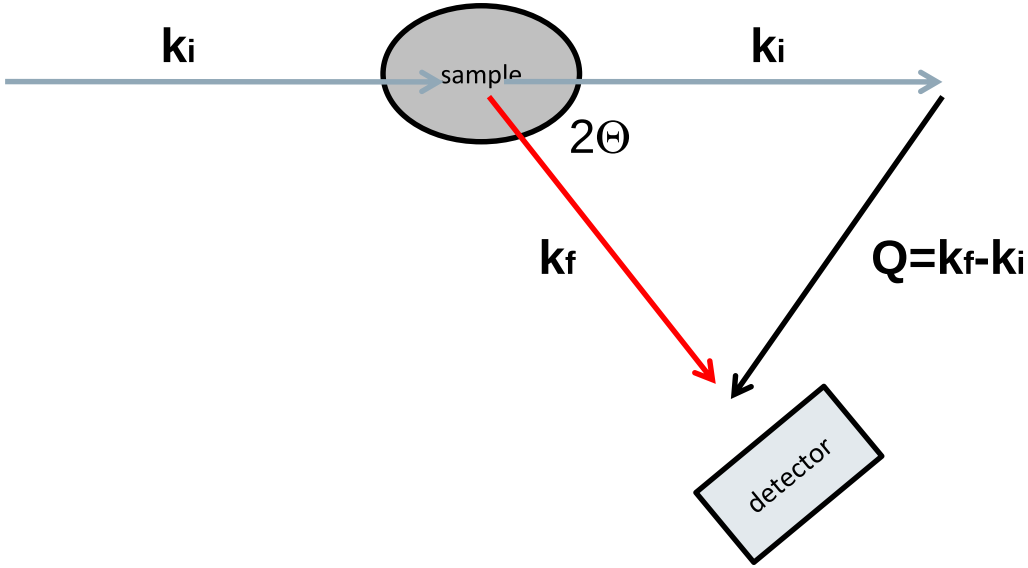
  $E_i = E_f$ vary 2Θ *(monochromatic)*

  vary $|E|$ fix 2Θ *(t.o.f.)*

- Quasi/in-elastic scattering:

  vary ω, normally Q will also change

  vary E_i or E_f and/or 2Θ



GENERIC INSTRUMENT

Energy selection

- How to measure the energy of a neutron beam?
- Or, how to monochromate a beam?
- Measure λ with Bragg reflection

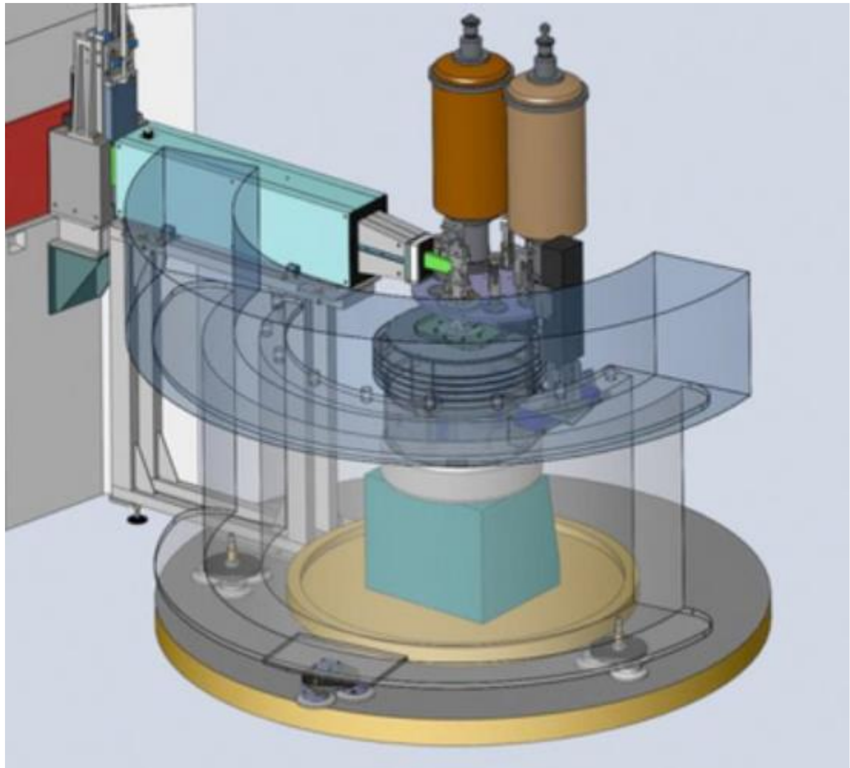
  $n\lambda = 2d\sin\Theta$

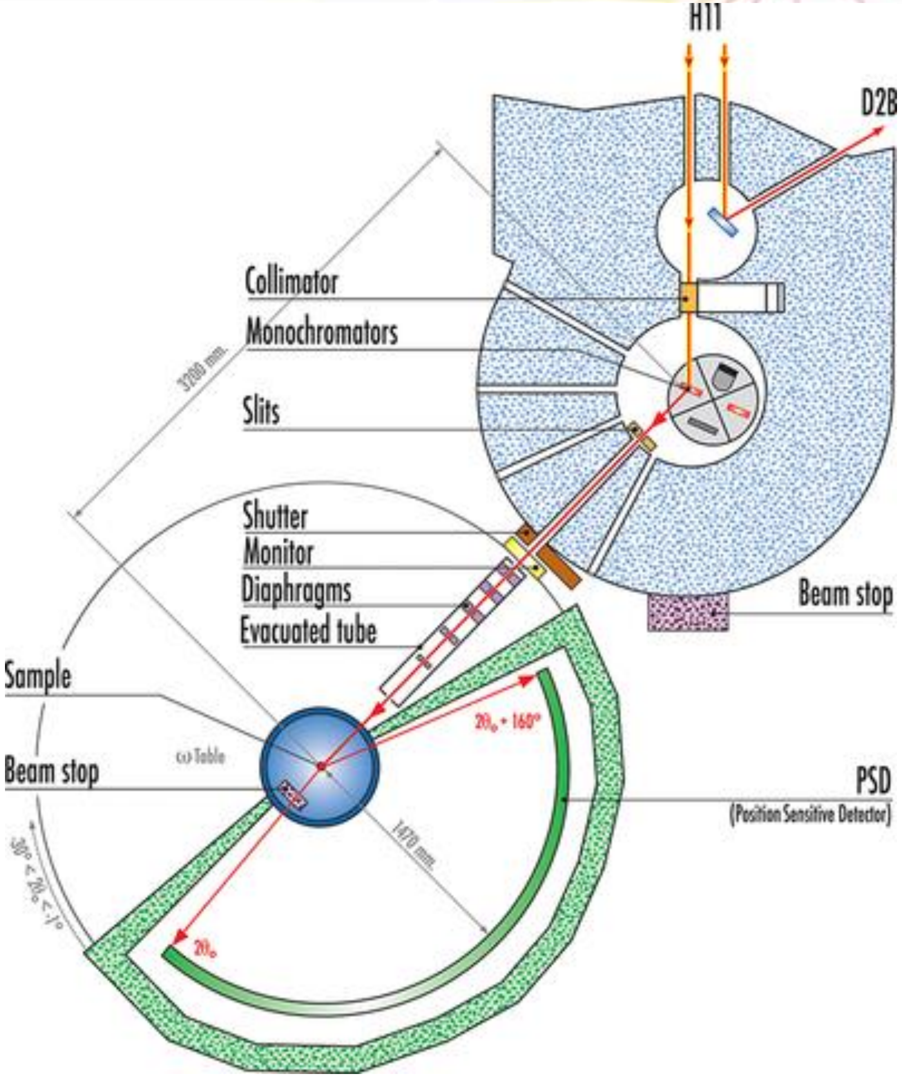
  d = distance between scattering planes
- Use neutron *t.o.f.* (or precession of neutron magnetic moments in a magnetic field)

$$tof = \frac{L}{v} = 253\mu\sec\cdot\lambda\left[\overset{o}{A}\right]\cdot L[m]$$

DIFFRACTION

Instruments (don’t measure the final energy!) – D2b & LADI

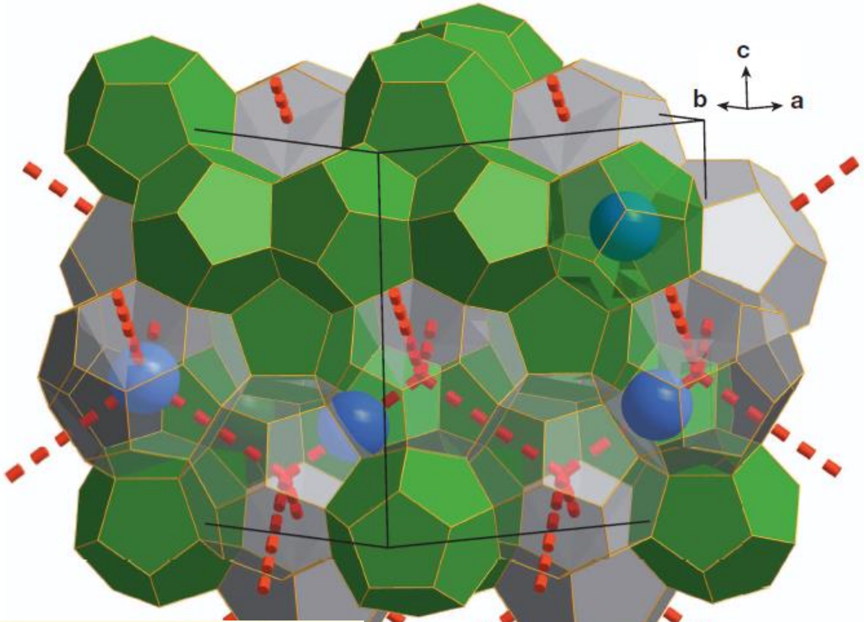


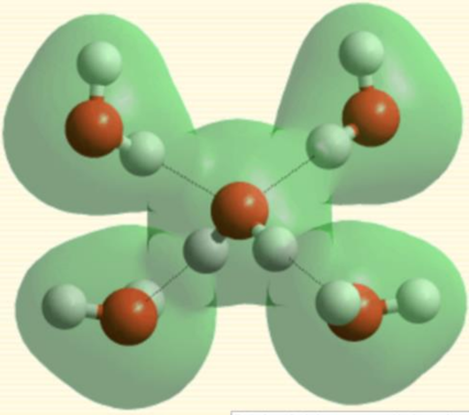


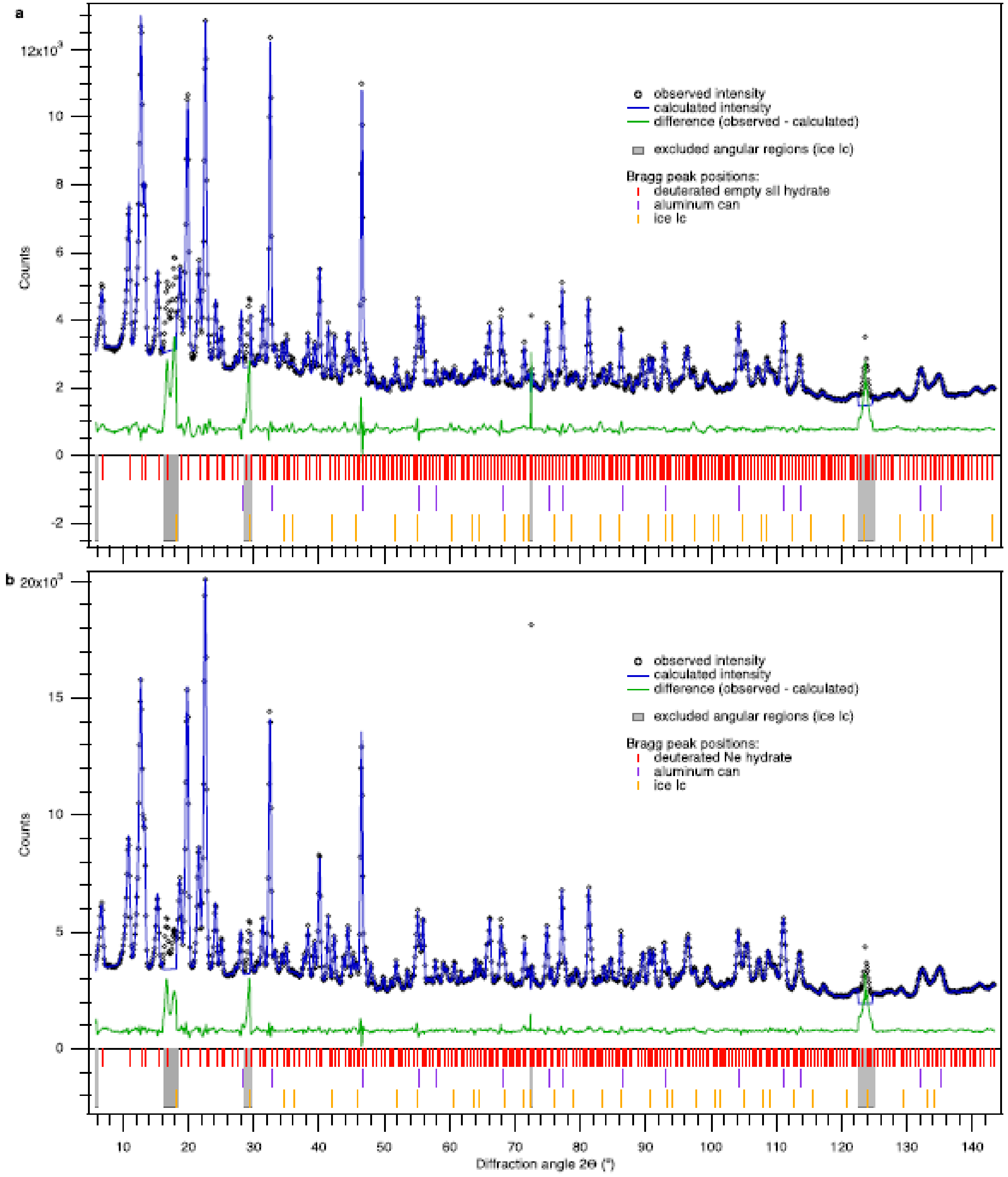
NEUTRONS
FOR SOCIETY

DIFFRACTION

Example – Formation and properties of ice XVI obtained by emptying a type sII clathrate hydrate





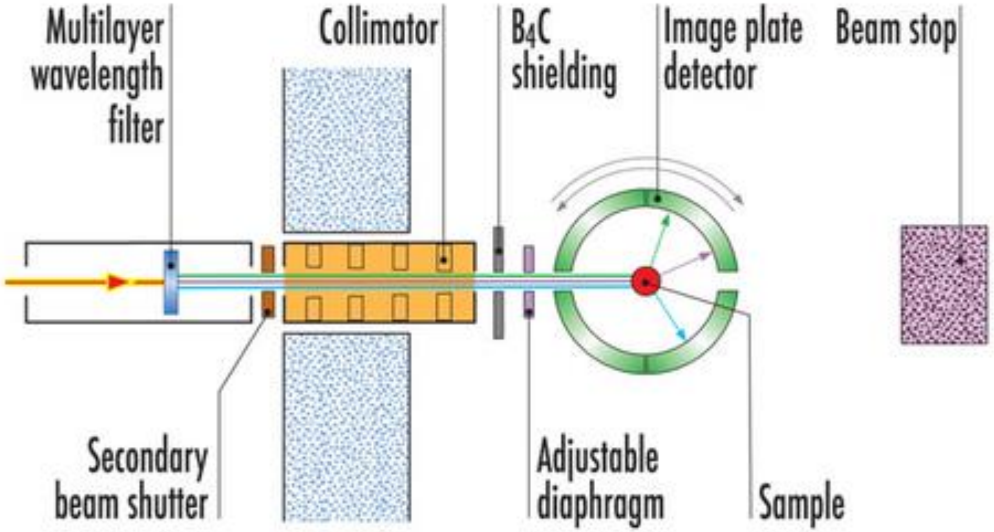


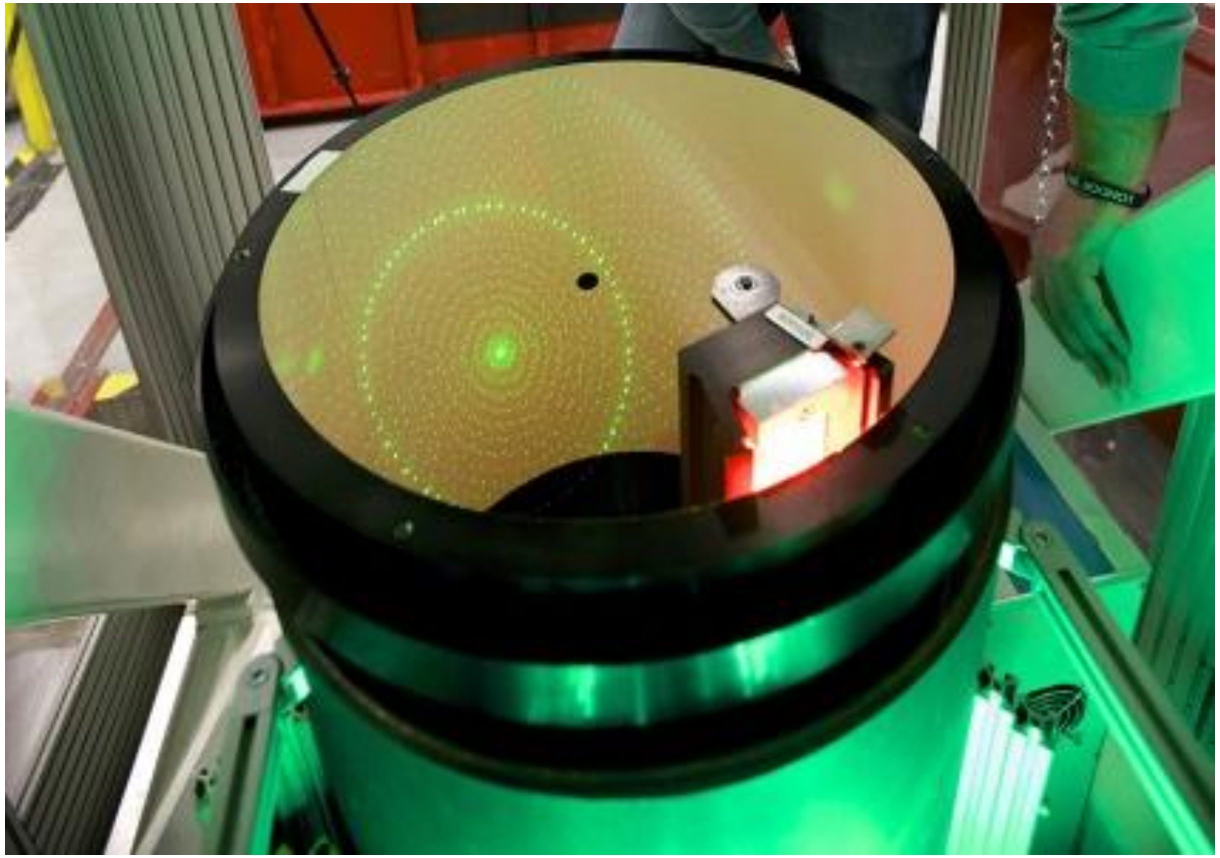
Extended Data Figure 2 | Diffraction patterns of Ne-filled and empty hydrate. **a**, **b**, Rietveld fit (obtained using FullProf software[32]) to diffraction pattern of empty sII D_2O hydrate (**a**) and Ne D_2O hydrate (**b**) taken at 5 K ($\lambda \approx 1.1226$ Å) on D20, ILL/Grenoble. The observed intensity is represented by open black circles, the calculated intensity as a blue line, the difference of both by a green line, grey shading marks the angular regions excluded in the refinement, red lines mark the positions of Bragg peaks of the hydrate, violet lines those of the aluminium sample can and orange lines those of ice Ic.

NEUTRONS
FOR SOCIETY

DIFFRACTION

Instruments (don't measure the final energy!) – D2b & LADI

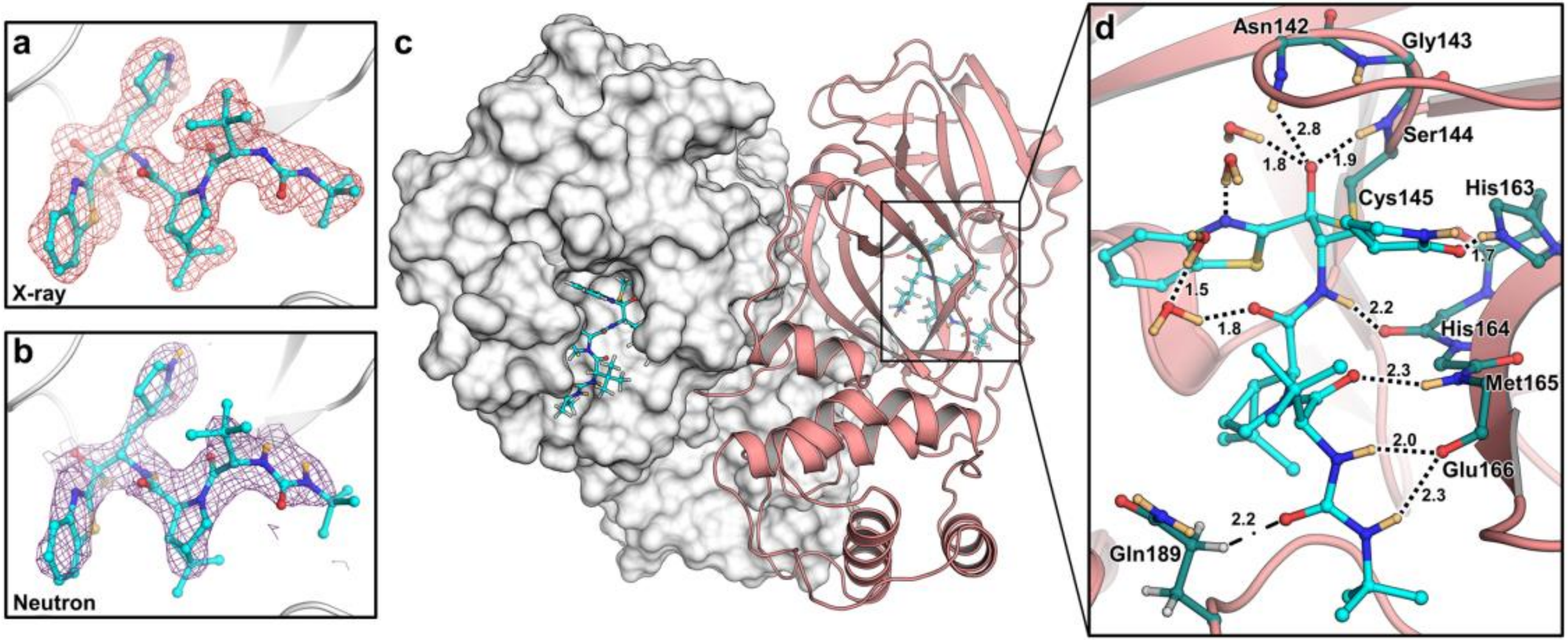




NEUTRONS FOR SOCIETY

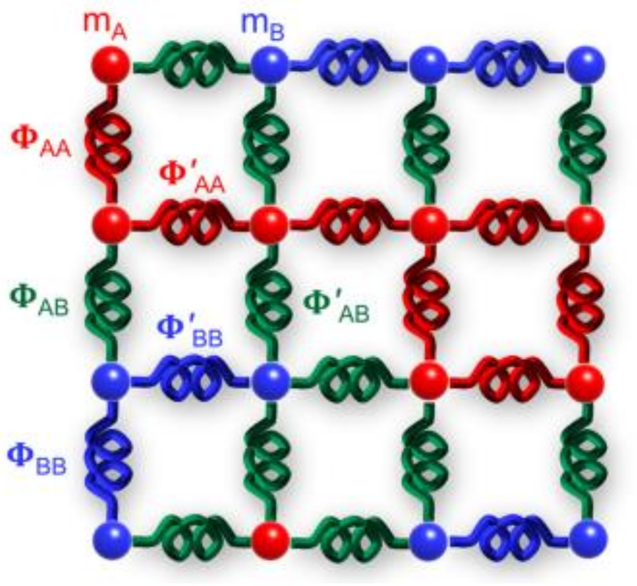
DIFFRACTION

Example – Improving drug design: SARS-COV2 Main Protease in complex with new clinical inhibitors (sample ~50 μg)



NEUTRONS FOR SOCIETY

SPECTROSCOPY – TIME/FREQUENCY DOMAIN



Simplified expressions for the scattering function – **coherent scattering**

When atoms move – vibrate around equilibrium positions

$R=R_0+\delta R(t)$

For normal modes: $\delta R(t)$ → displacement vectors ***e*** & frequencies ω

Coherent scattering - Phonons:

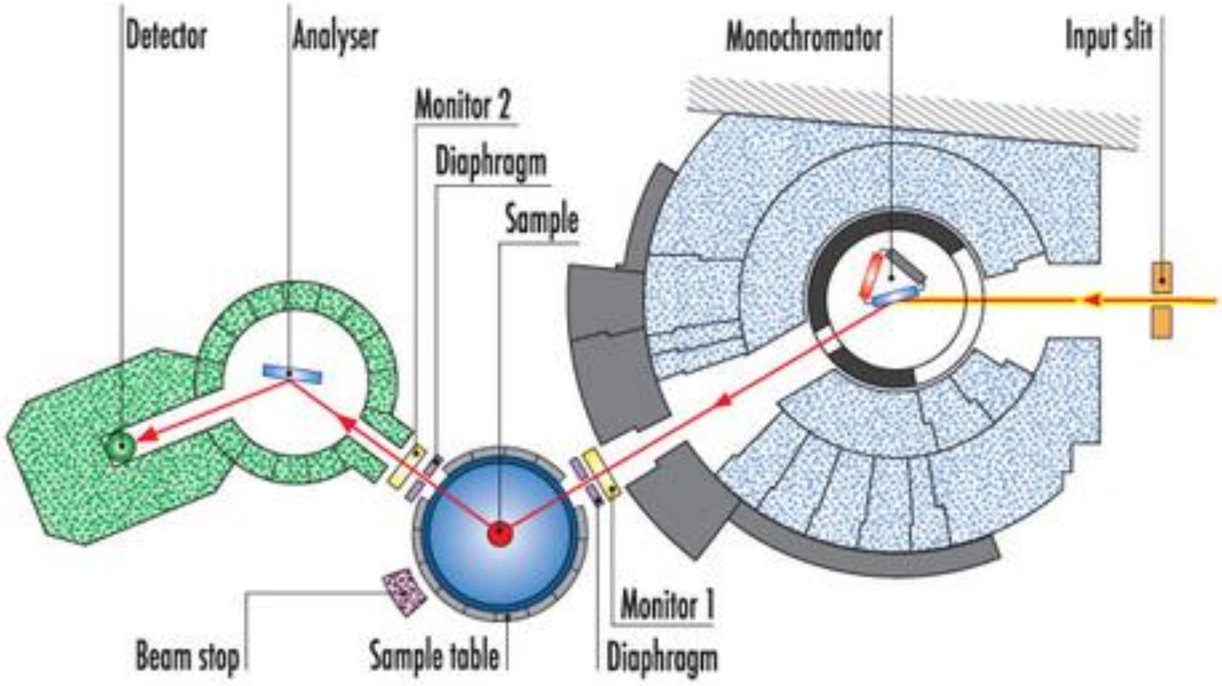
- Short range coupling gives long range correlations
- Dispersion as a function of ***q*** (or wavelength) – guitar string!

$$\left.\frac{d^2\sigma}{d\Omega dE_f}\right)_{coh\pm1} = \frac{\sigma_{coh}}{4\pi}\frac{k_f}{k_i}\frac{(2\pi)^3}{v_0}\frac{1}{2M}\exp(-2W)\sum_s\sum_\tau \frac{\left(\vec{Q}\cdot\vec{e}_s\right)}{\omega_s}\left\langle n_s+1/2\pm1/2\right\rangle$$

$$\times\delta(\omega\mp\omega_s)\,\delta\left(\vec{Q}\mp\vec{q}-\vec{\tau}\right)$$

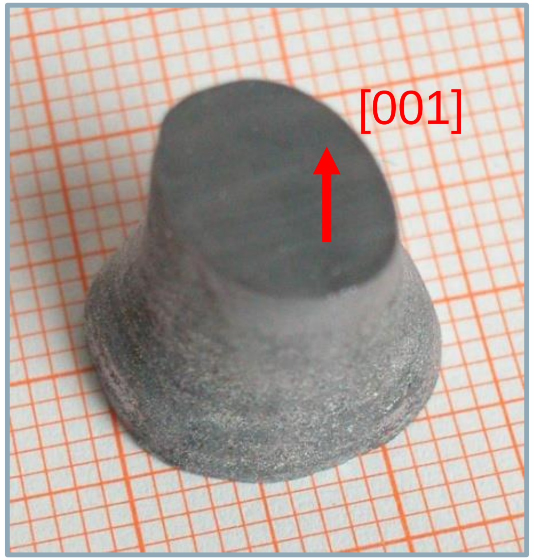
SPECTROSCOPY – TIME/FREQUENCY DOMAIN

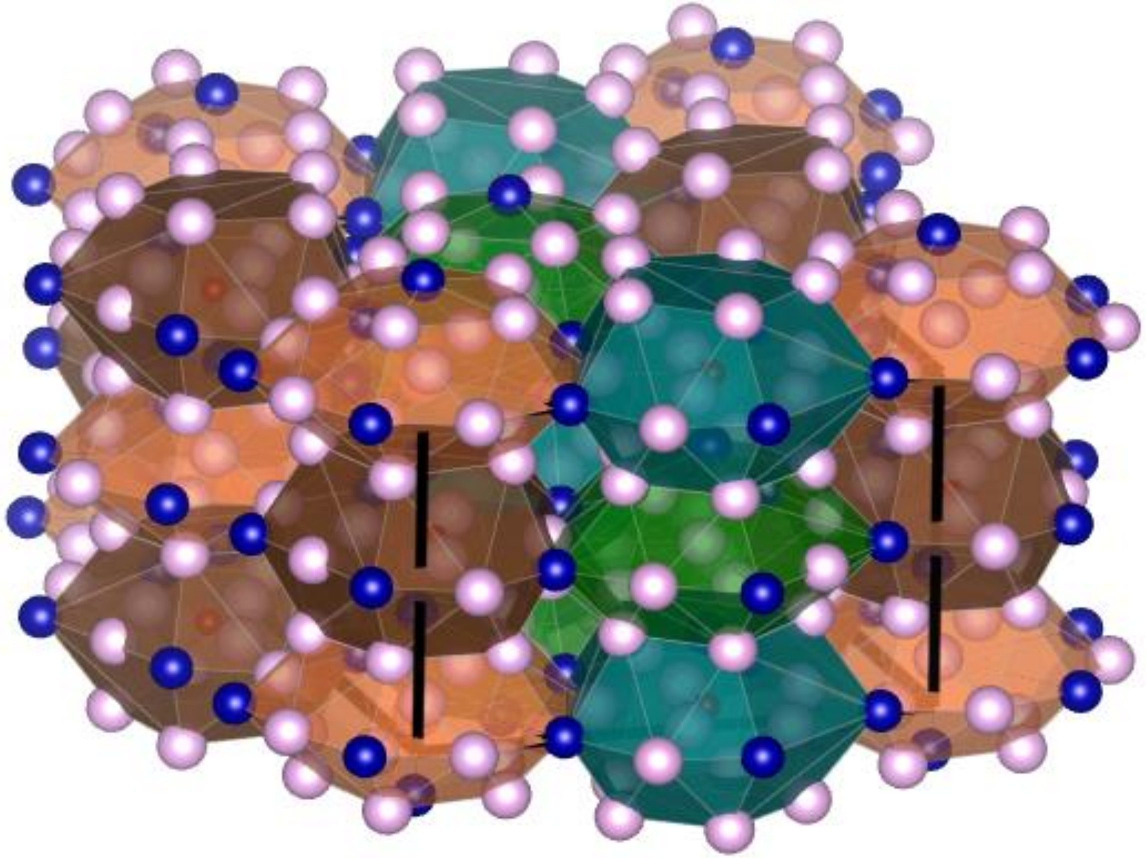
Instruments – varying k_i & k_f – TAS, TOF



SPECTROSCOPY – TIME/FREQUENCY DOMAIN

Example – heat gradient (low thermal conductivity – short phonon paths and lifetimes) generates current in thermoelectrics - Complex Metallic Alloy - $Al_{13}Co_4$ Quasicrystal approximant





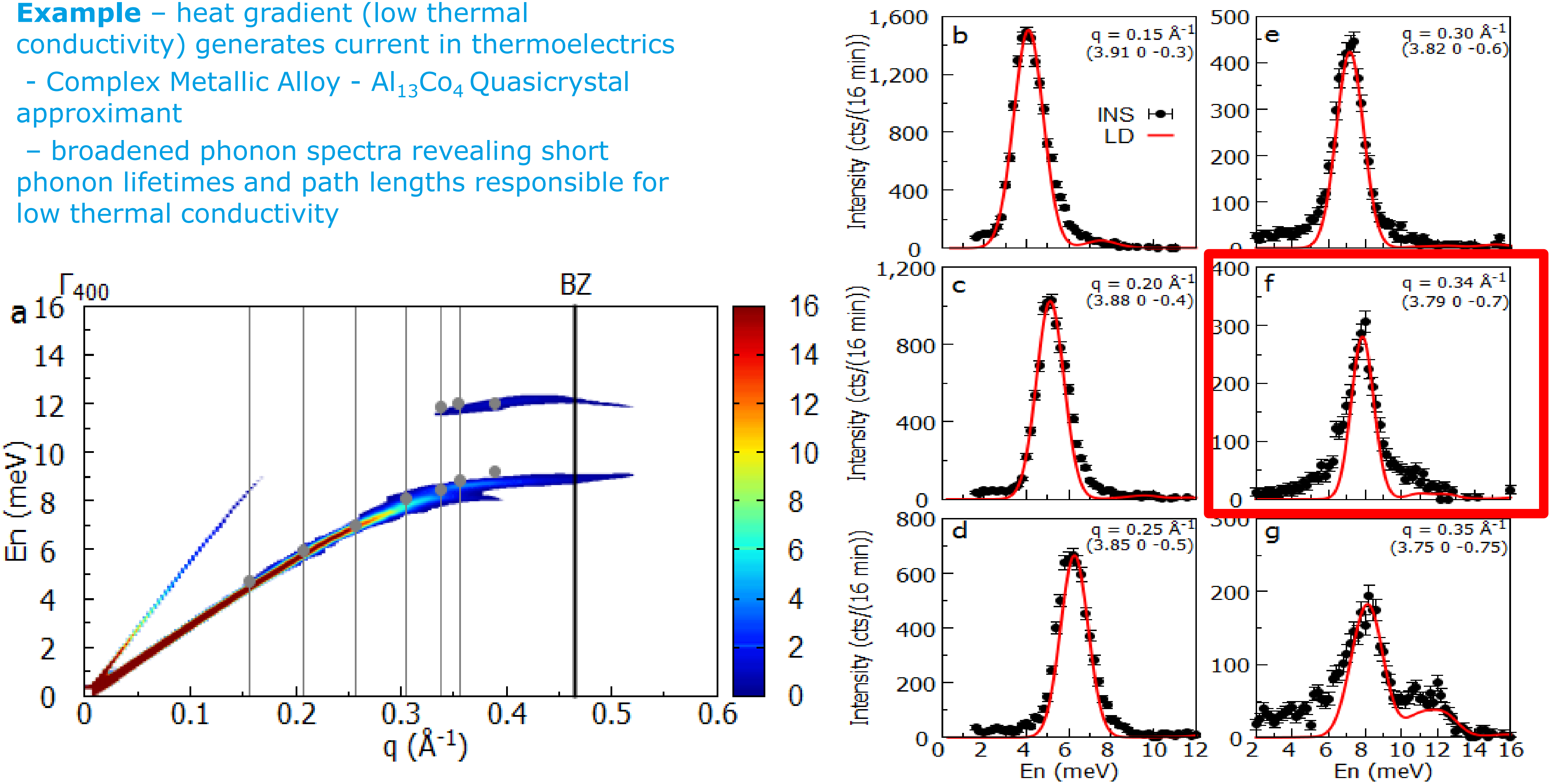
NEUTRONS FOR SOCIETY

SPECTROSCOPY – TIME/FREQUENCY DOMAIN

Example – heat gradient (low thermal conductivity) generates current in thermoelectrics

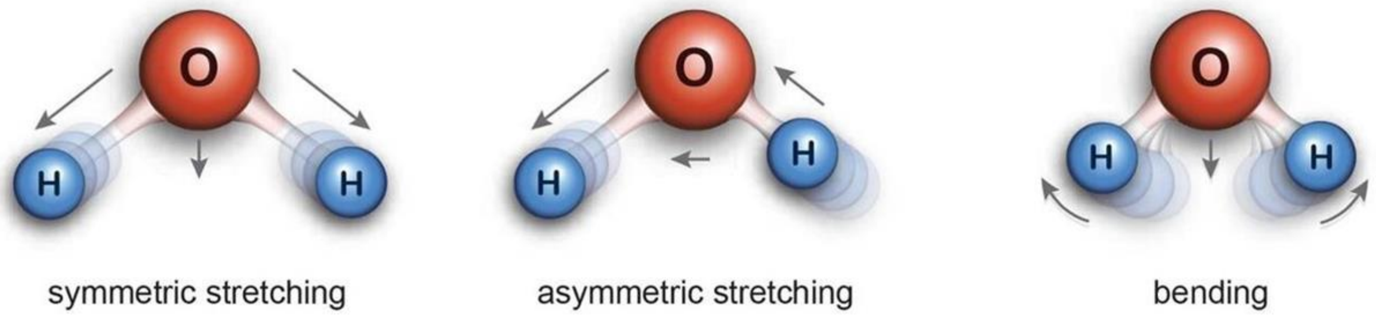
- Complex Metallic Alloy - $Al_{13}Co_4$ Quasicrystal approximant

– broadened phonon spectra revealing short phonon lifetimes and path lengths responsible for low thermal conductivity



SPECTROSCOPY – TIME/FREQUENCY DOMAIN

Simplified expressions for the scattering function
– **incoherent scattering**


symmetric stretching

asymmetric stretching

bending

For atoms that vibrate around equilibrium positions

$R=R_0+\delta R(t)$

For normal modes: $\delta R(t)$ → displacement vectors ***e*** & frequencies ω

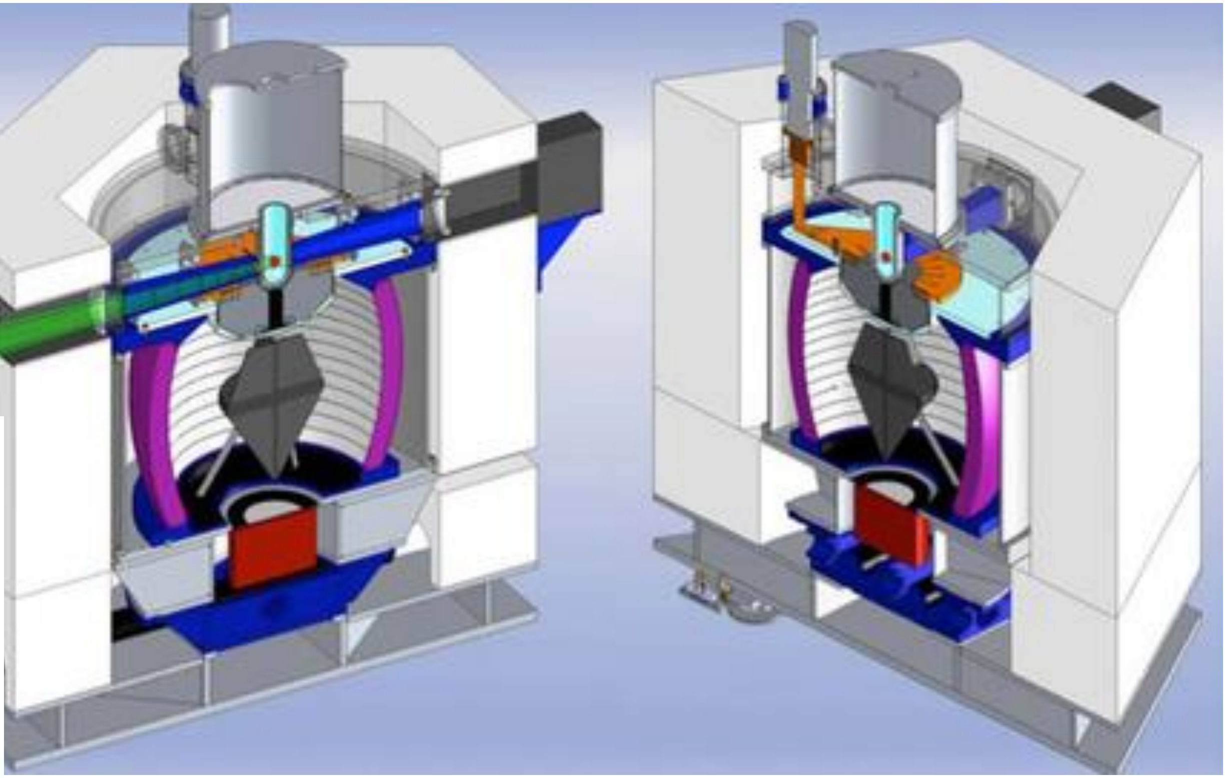
Incoherent scattering - Internal (molecular) modes:

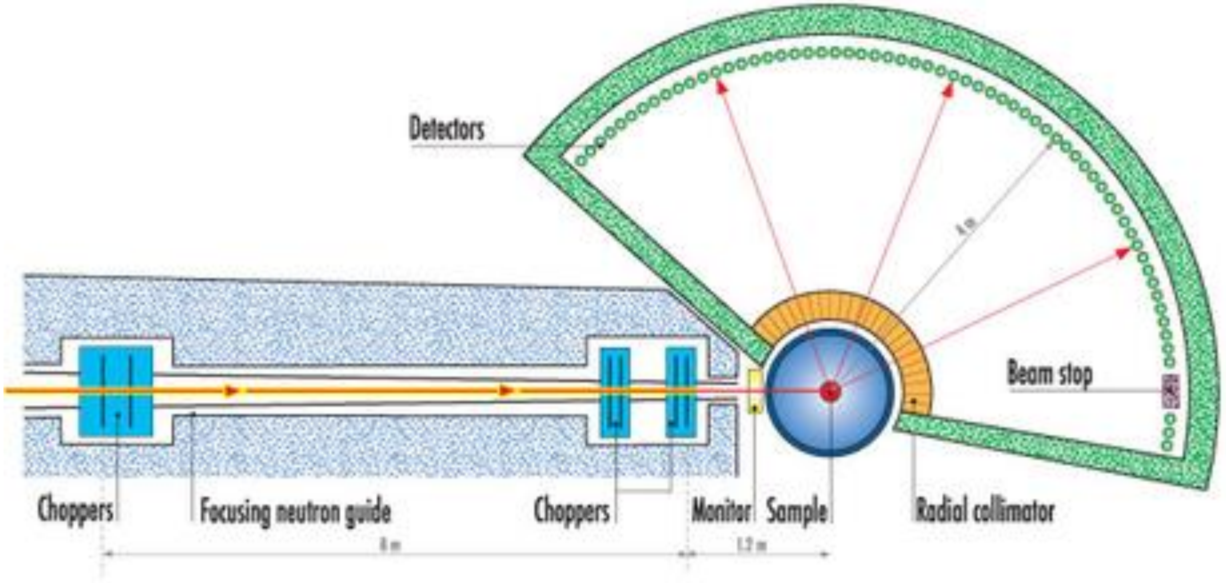
- No long range correlations due to weak coupling
- No dispersion

$$\left.\frac{d^2\sigma}{d\Omega dE_f}\right)_{incoh\pm1}=\frac{k_f}{k_i}\sum_s \delta(\omega\mp\omega_s)\frac{\langle n_s+1/2\pm1/2\rangle}{2\omega_s}\sum_r\frac{(\sigma_{incoh})_r}{4\pi}\frac{1}{M_r}\left|\vec{Q}\cdot\vec{e}_r\right|^2\exp(-2W_r)$$

SPECTROSCOPY – TIME/FREQUENCY DOMAIN

Instruments – TOF, Lagrange
(direct & indirect spectrometers
- fixed incident/final energies
respectively)

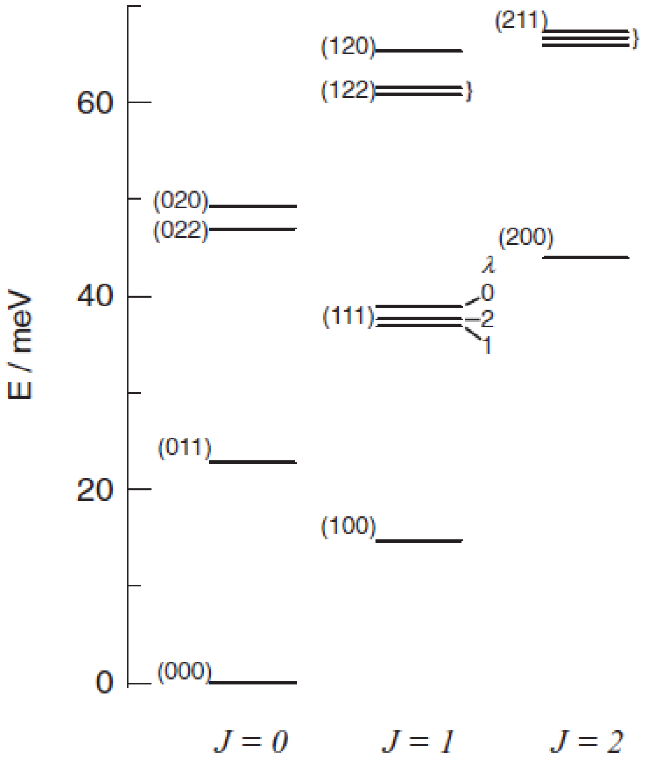


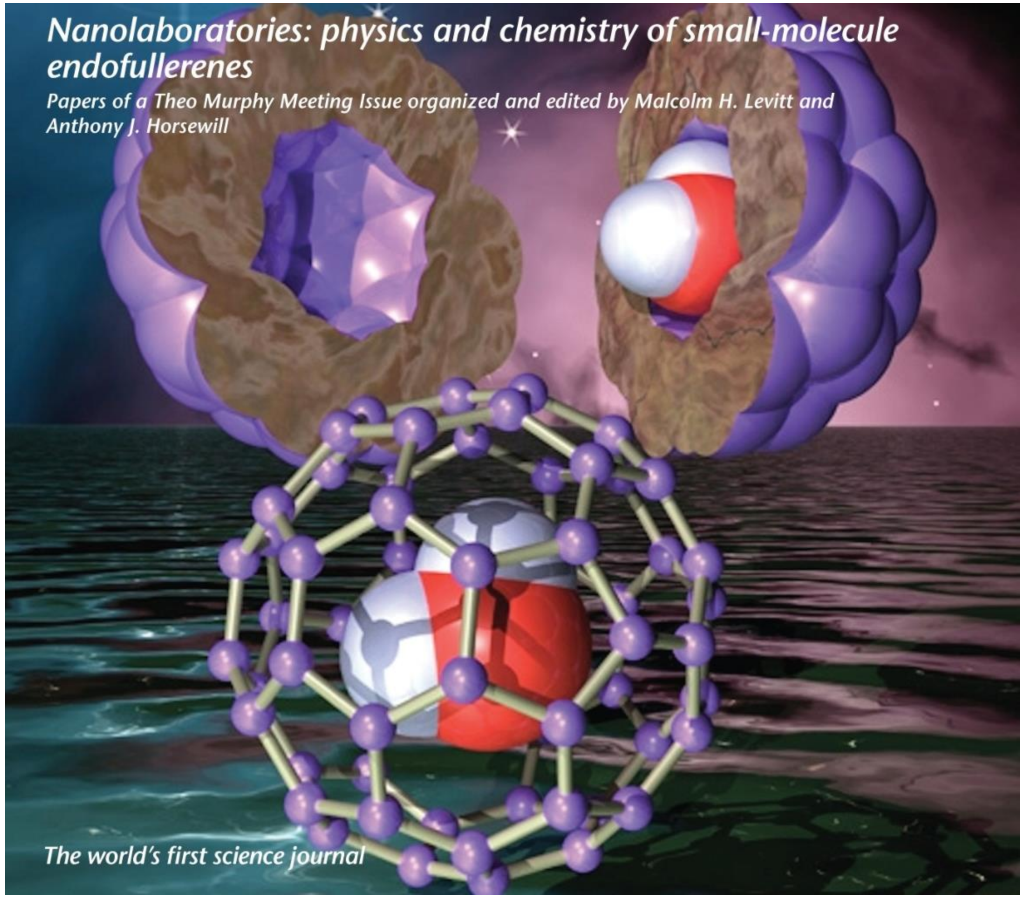


SPECTROSCOPY – TIME/FREQUENCY DOMAIN

Example – endofullerenes – a molecular nanolab

(Molecular spectroscopy – no dispersion but useful Q-dependence)





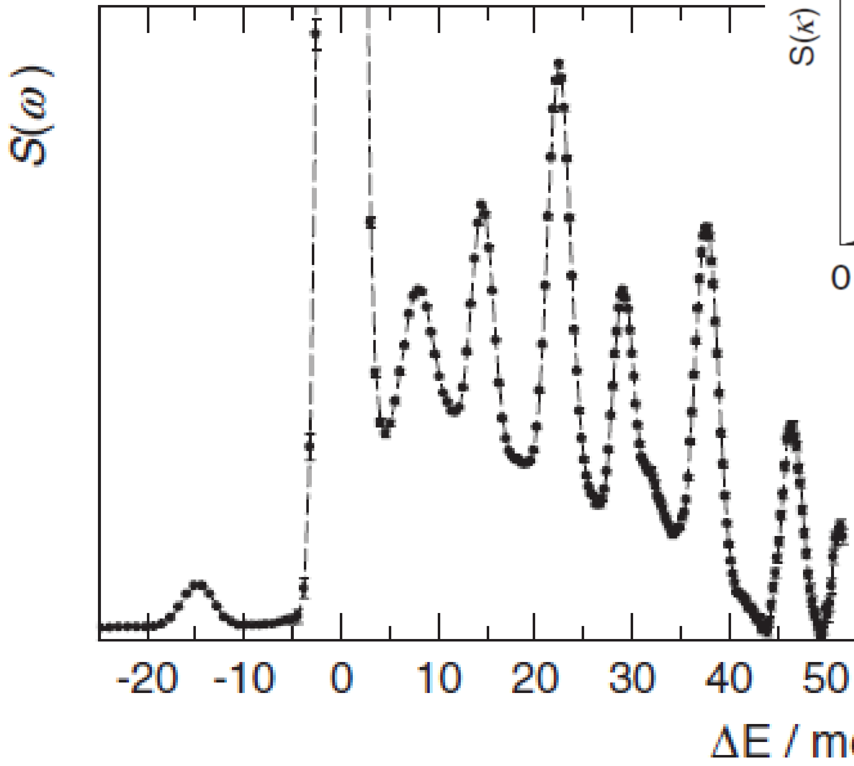
Nanolaboratories: physics and chemistry of small-molecule endofullerenes

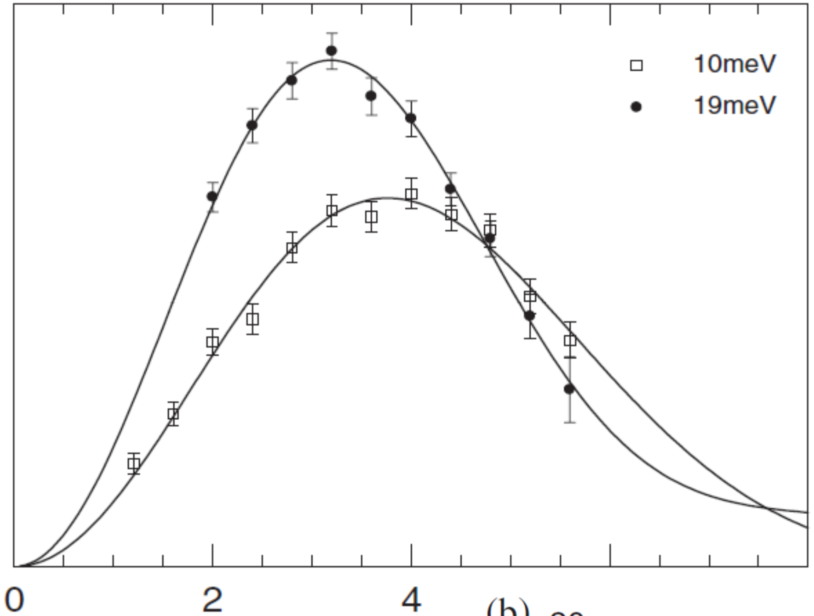
Papers of a Theo Murphy Meeting Issue organized and edited by Malcolm H. Levitt and Anthony J. Horsewill

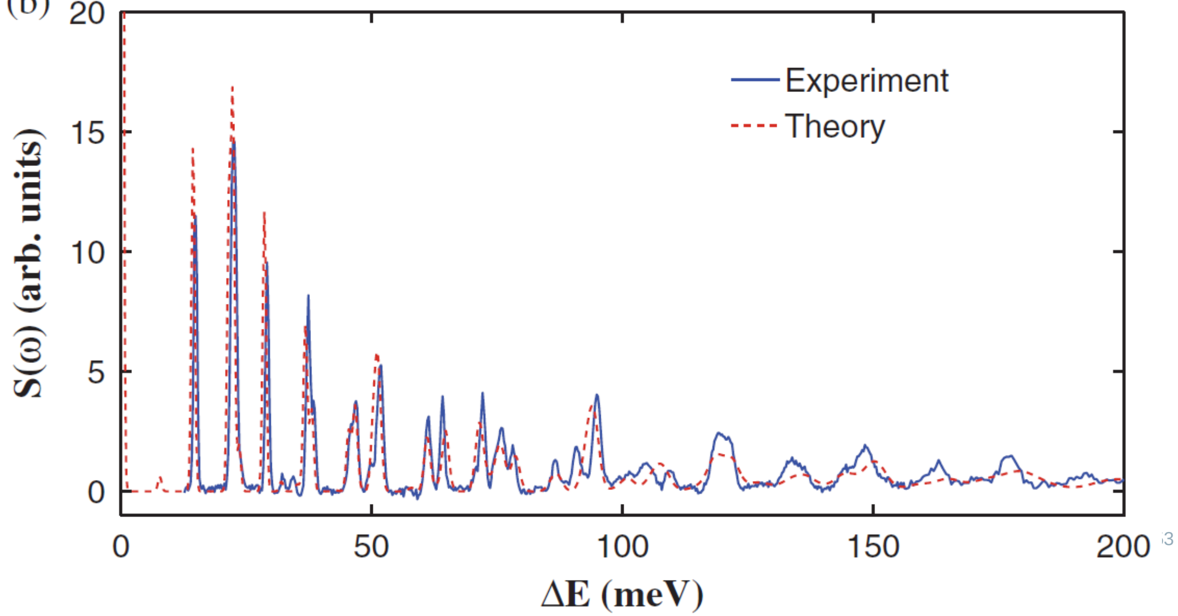
The world's first science journal

SPECTROSCOPY – TIME/FREQUENCY DOMAIN

Example – endofullerenes

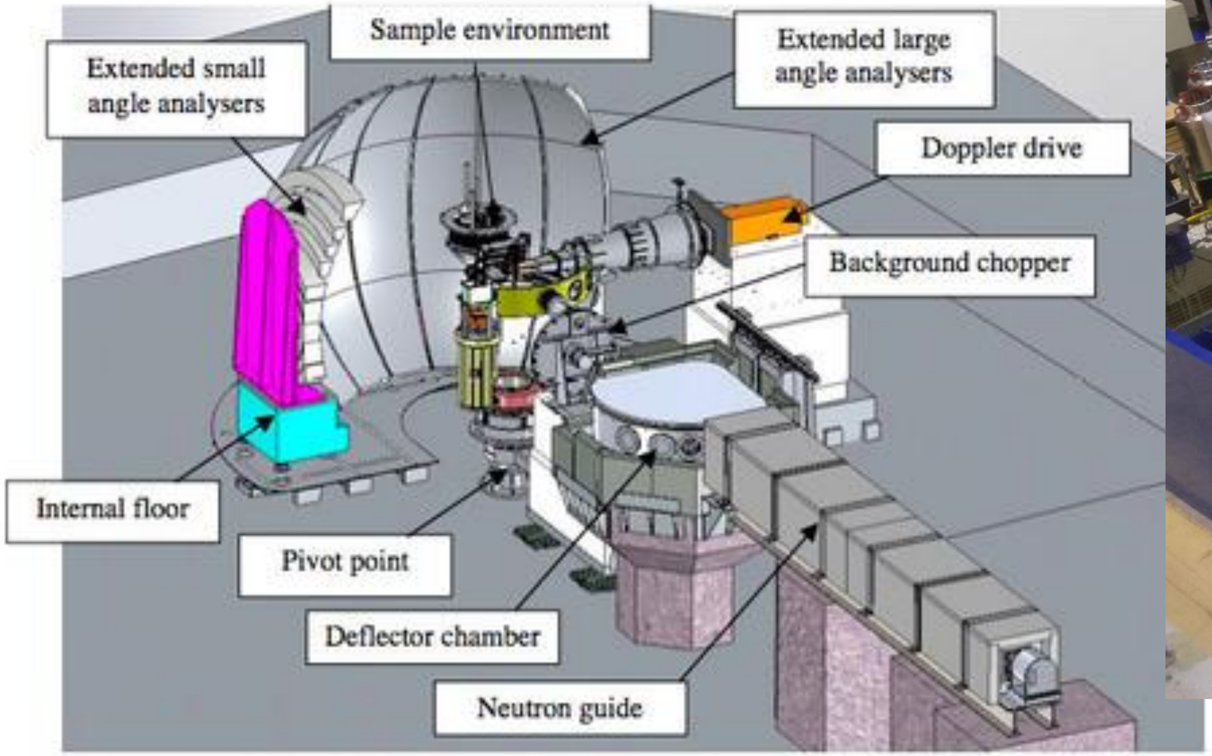


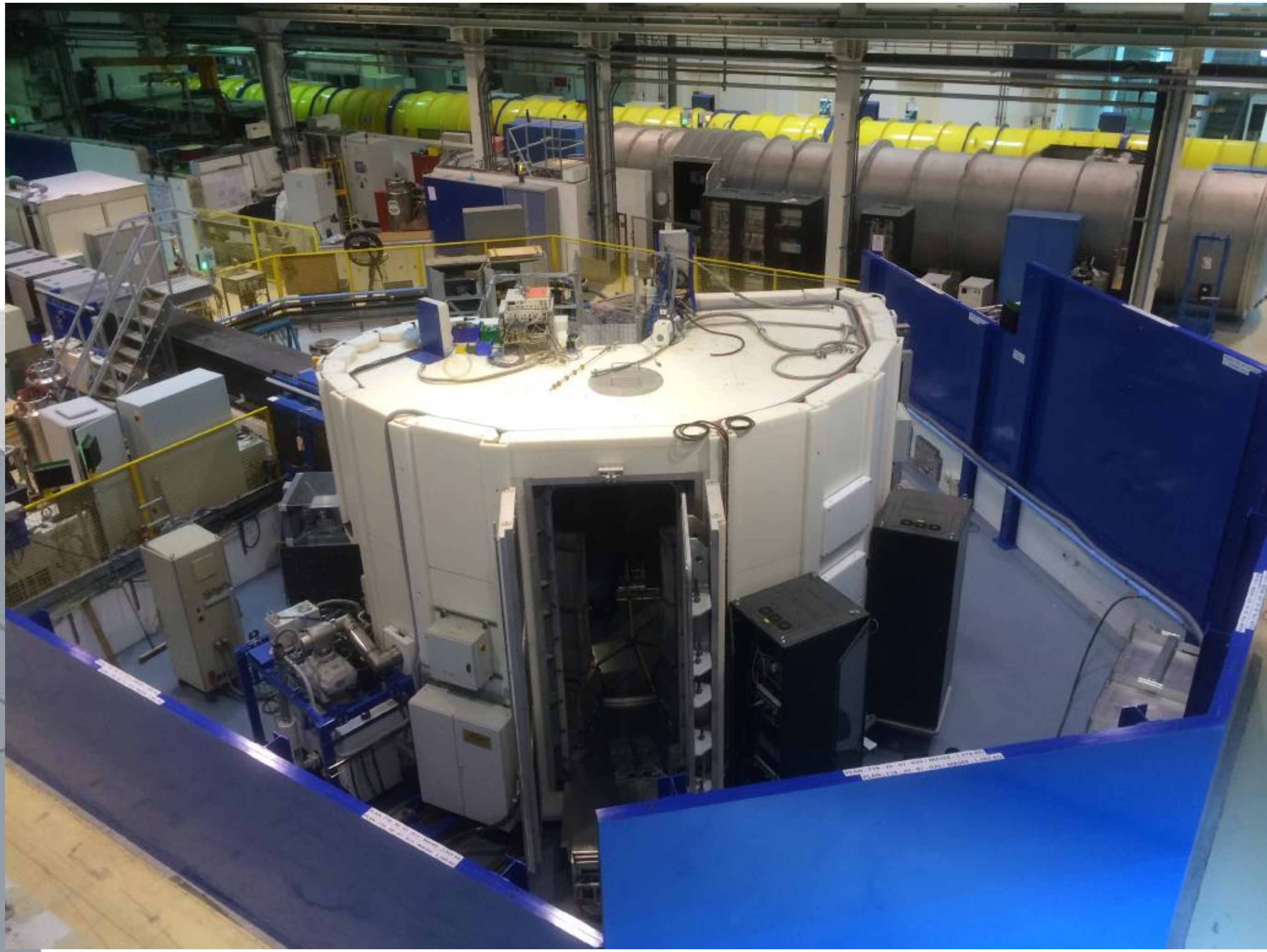




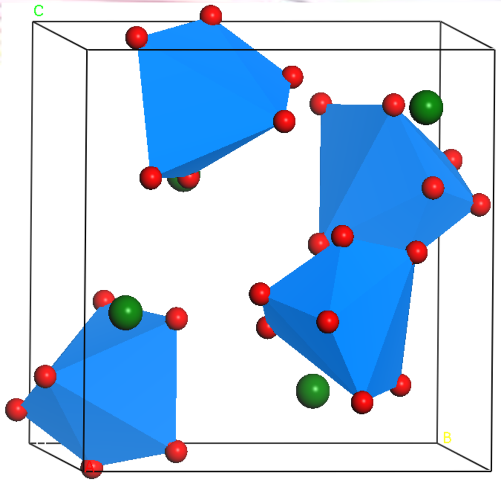
SPECTROSCOPY – TIME/FREQUENCY DOMAIN

Instruments – Back-Scattering

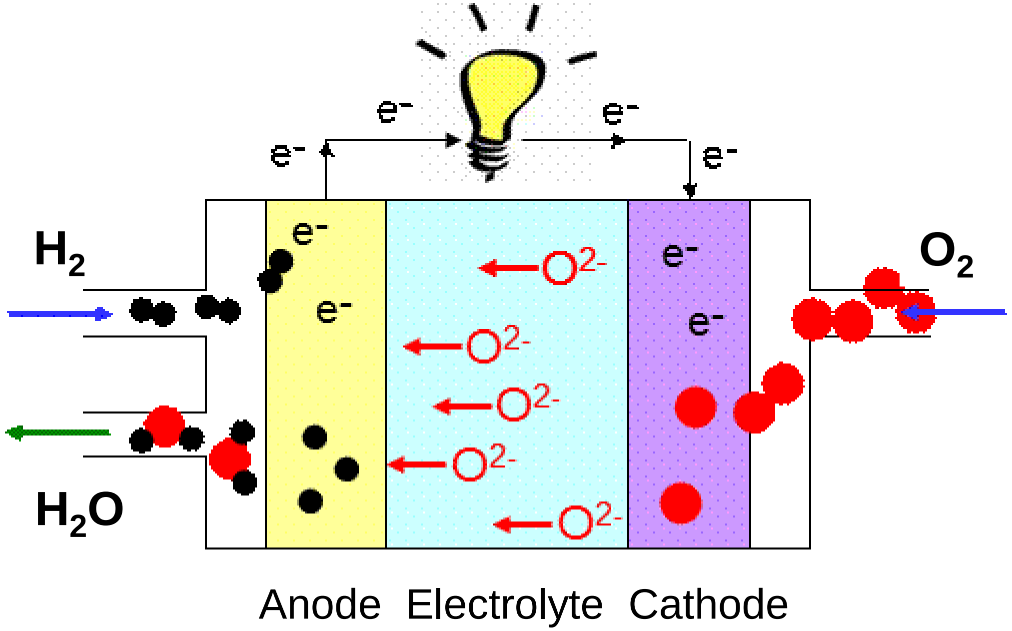


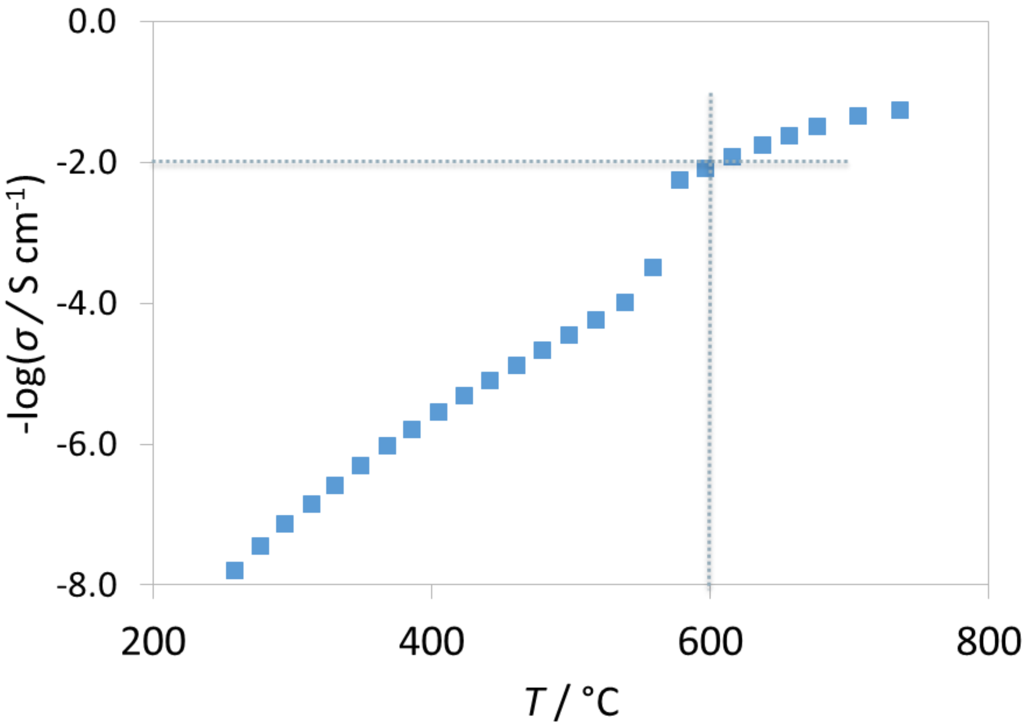


SPECTROSCOPY – TIME/FREQUENCY DOMAIN



Example – oxide ion conductors
Diffusion of oxygen ions through an electrolyte
Measured as a 'Doppler broadening' of the elastic peak
→ quasielastic scattering



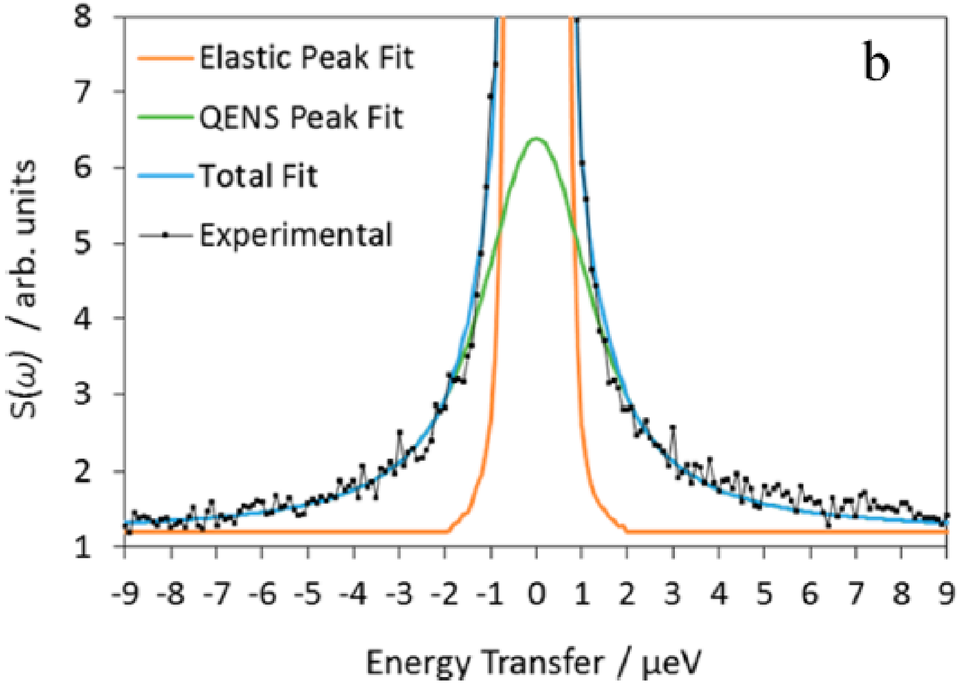


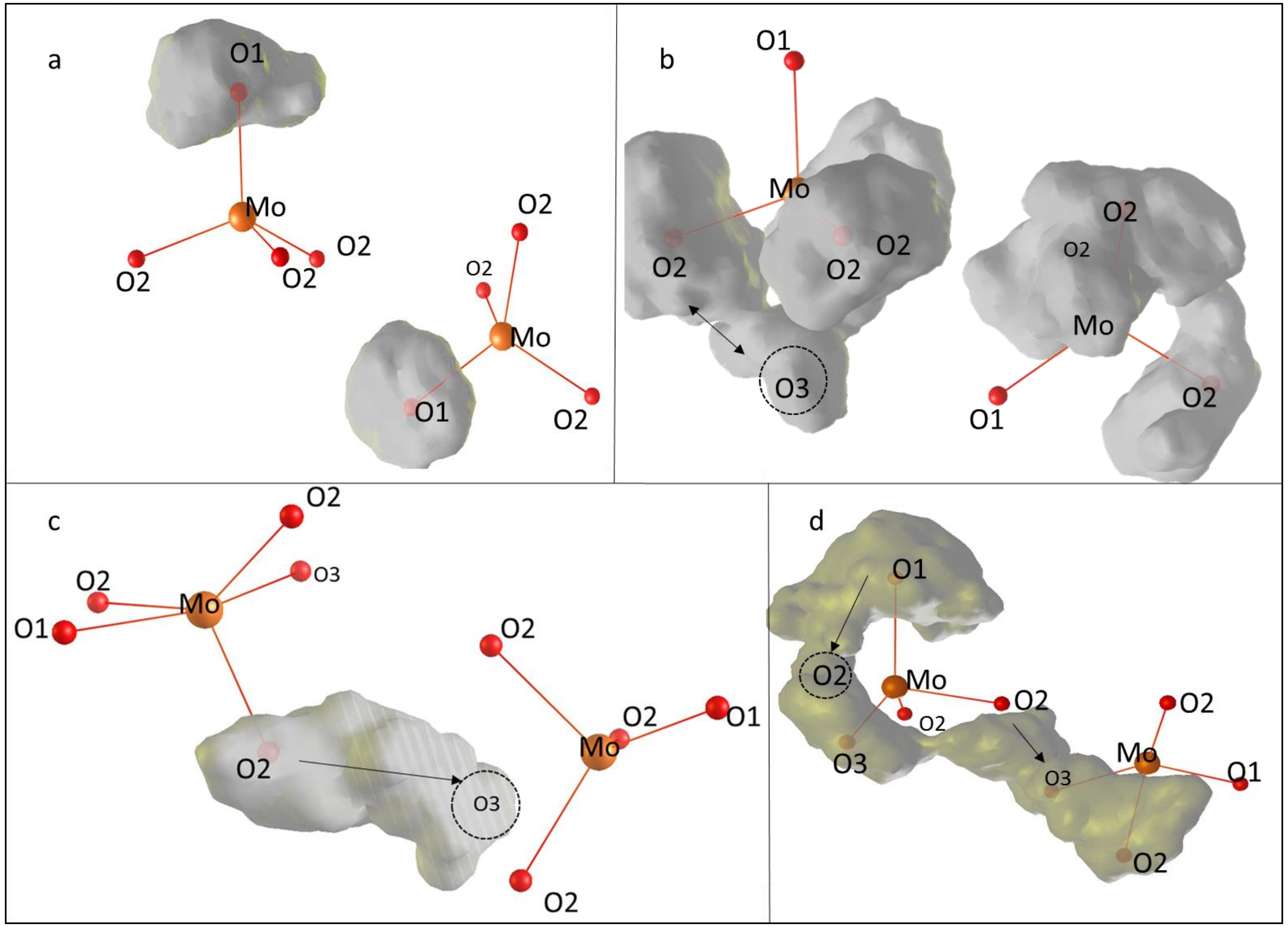
NEUTRONS FOR SOCIETY

SPECTROSCOPY – TIME/FREQUENCY DOMAIN

Example – oxide ion conductors

Quasielastic scattering reveals ionic pathways
– details from molecular dynamics

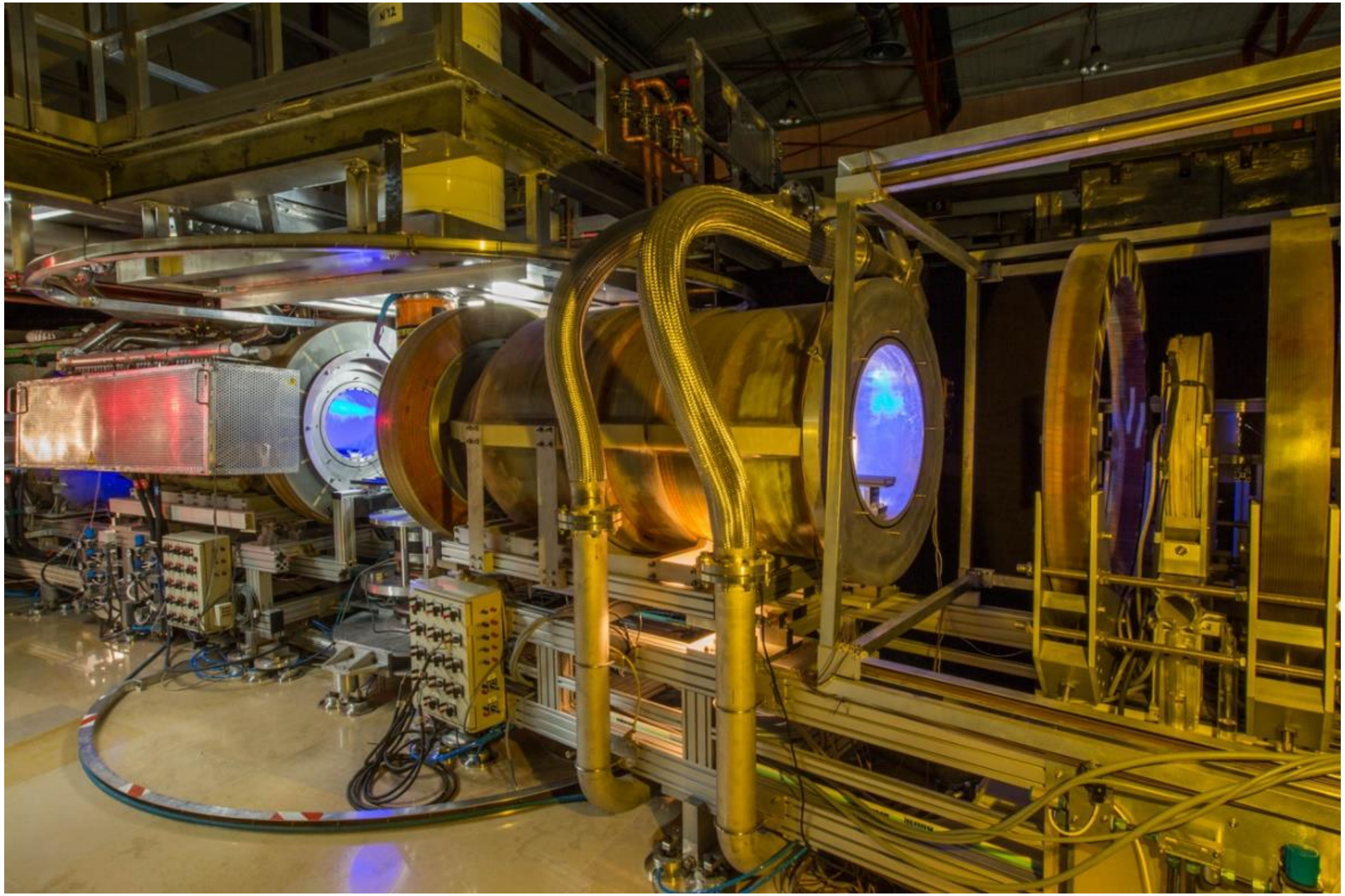




NEUTRONS FOR SOCIETY

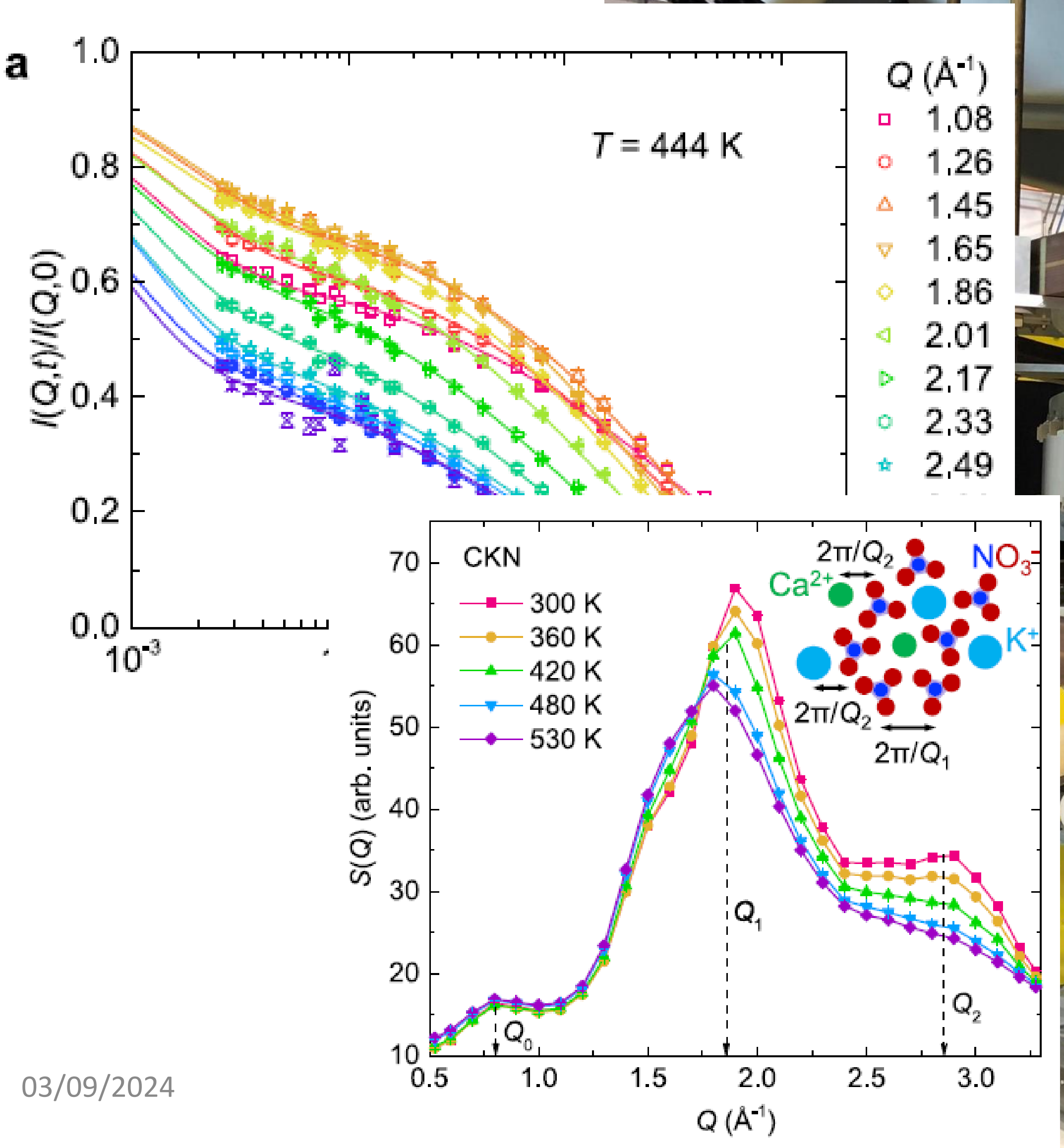
SPECTROSCOPY – SPIN ECHO

Energy selection - precession of neutron magnetic moments in a magnetic field (depends on t.o.f. in B)



NEUTRONS
FOR SOCIETY

SPECTROSCOPY – SPIN ECHO



03/09/2024

MAGNETISM

Structure and dynamics – double differential cross-section

As for interactions with nuclei but

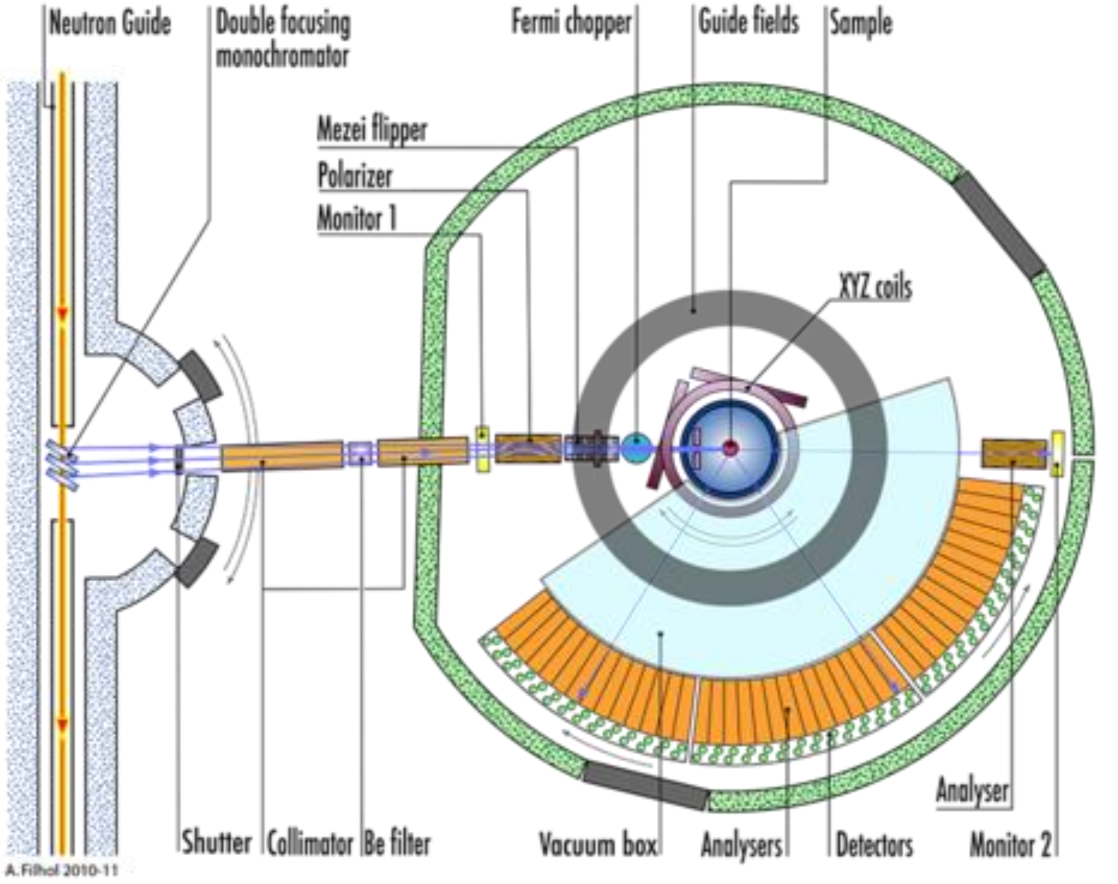
- Neutron spin probes local magnetic fields due to electron spin and orbital contribution
- Atomic form factor – scattering from an atom is angular dependent due to electron cloud
- No incoherence effects
- N.B. σ and V in these equations

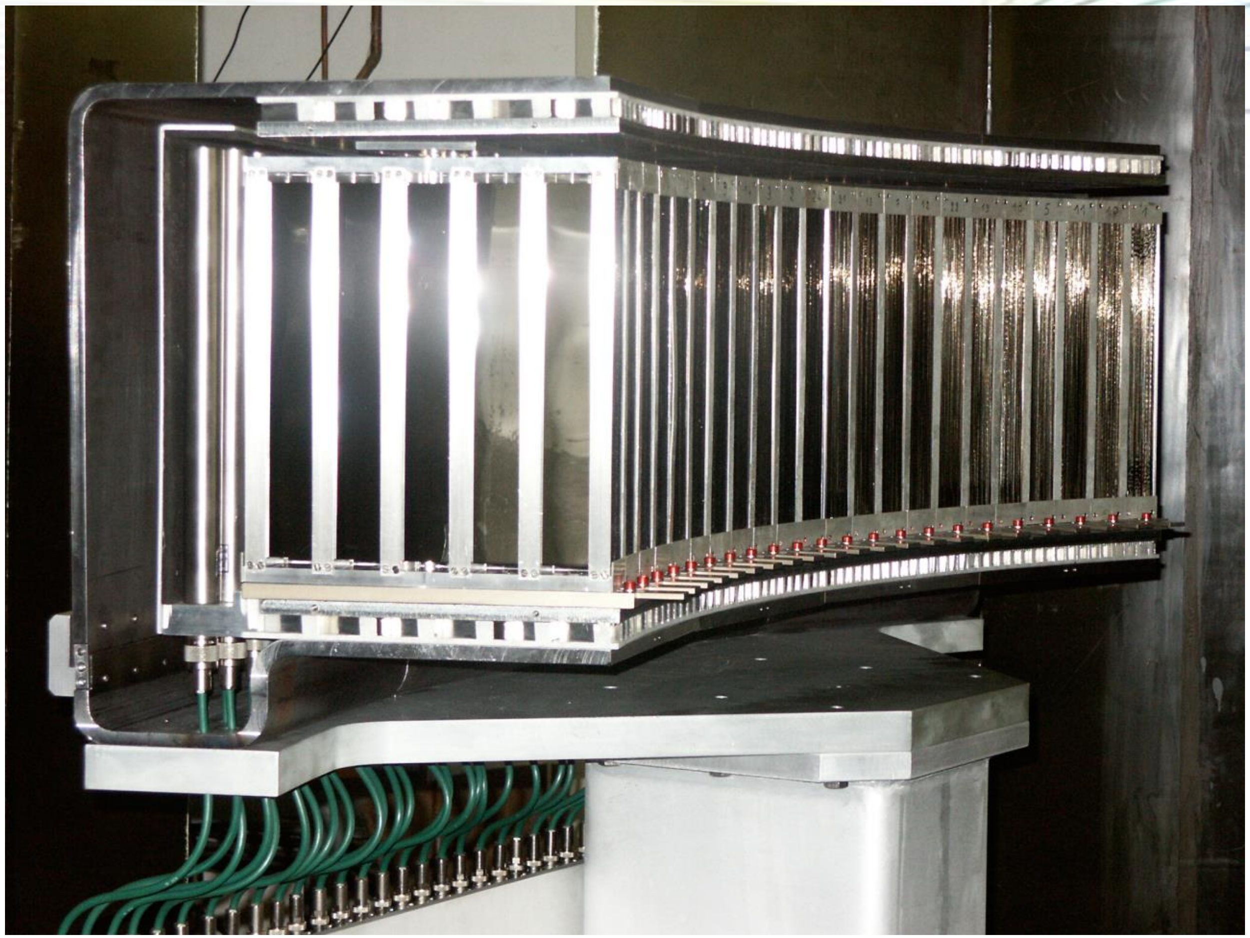
$$V_m = -\mu_n \cdot B = -\frac{\mu_0}{4\pi}\gamma\mu_N 2\mu_B\left\{curl\left(\frac{s\times R}{R^2}\right)+\frac{1}{\hbar}\frac{p\times R}{R^2}\right\}$$

$$\left(\frac{d^2\sigma}{dE_f\,d\Omega}\right)_{\sigma_i\lambda_i\to\sigma_f\lambda_f} = \frac{k_f}{k_i}\left(\frac{m_n}{2\pi\hbar^2}\right)^2\left|\left\langle k_f\sigma_f\lambda_f\middle|V_m\middle|k_i\sigma_i\lambda_i\right\rangle\right|^2\delta\left(E_i - E_f + E_{\lambda_i} - E_{\lambda_f}\right)$$

MAGNETISM

Polarised neutrons – separate nuclear and magnetic signals & more precise information on magnetic structures



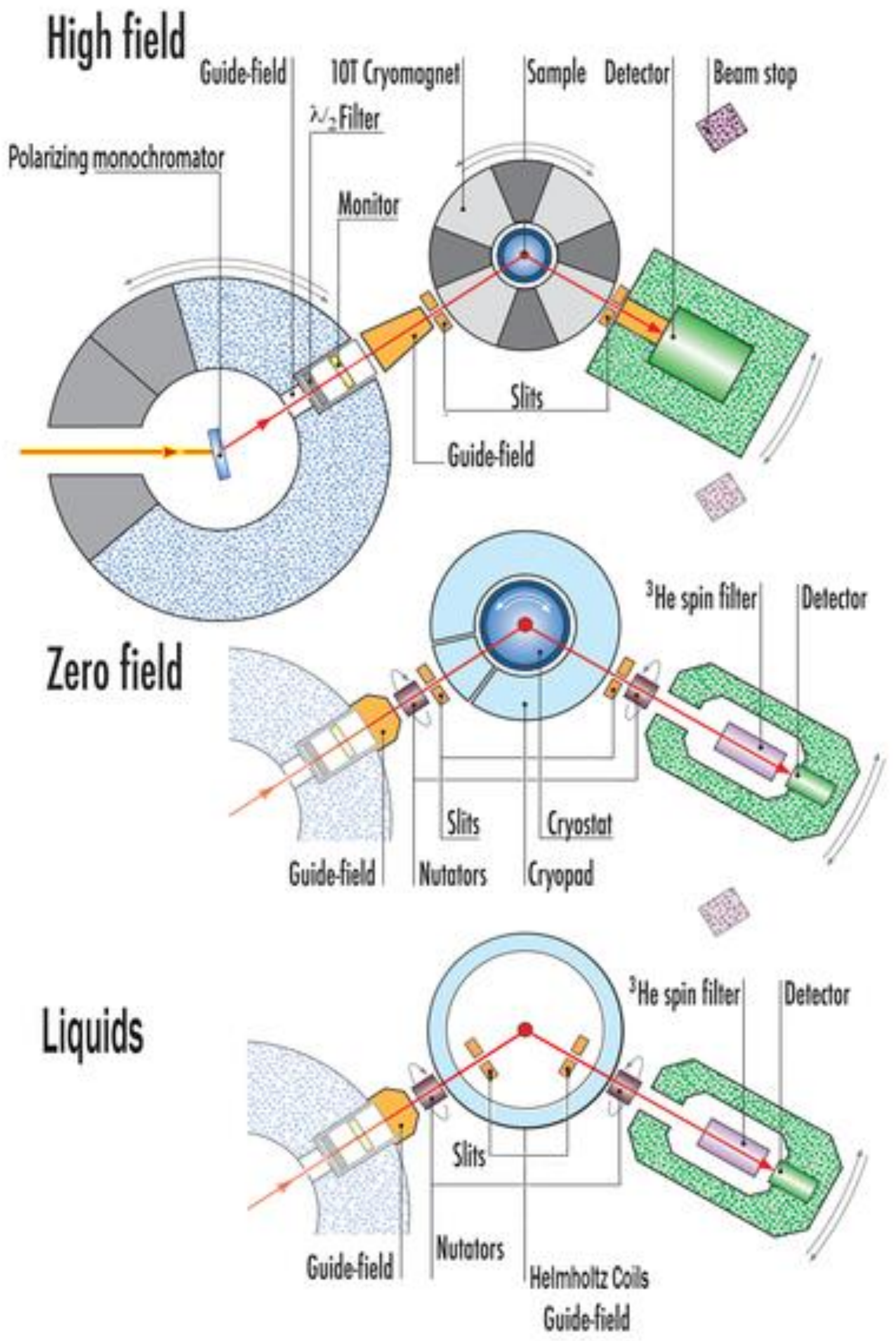


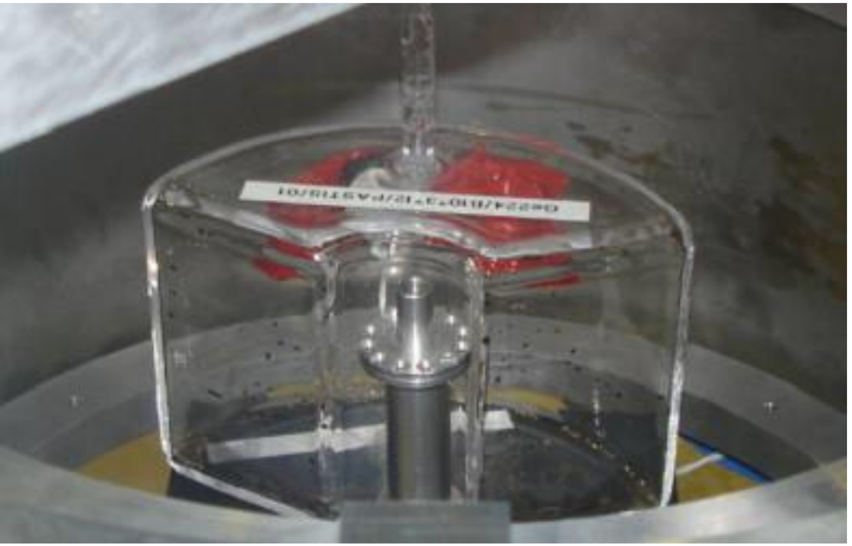
- Measure 2, 6 or 10 polarised scattering channels: u→u (non spin flip) and d→u (spin flip) in the simplest case

MAGNETISM

Polarised neutrons – separate nuclear and magnetic signals
& more precise information on magnetic structures

- Polarised (optically pumped) 3He selectively absorbs one neutron spin state – more versatile polariser
- Cryopad allows full control of incident and scattered neutron polarisation – spherical polarimetry





MAGNETISM

EXAMPLE - SPHERICAL NEUTRON POLARIMETRY TO STUDY MAGNETOELECTRIC CuFeO_2 – **0.04 mm^3**

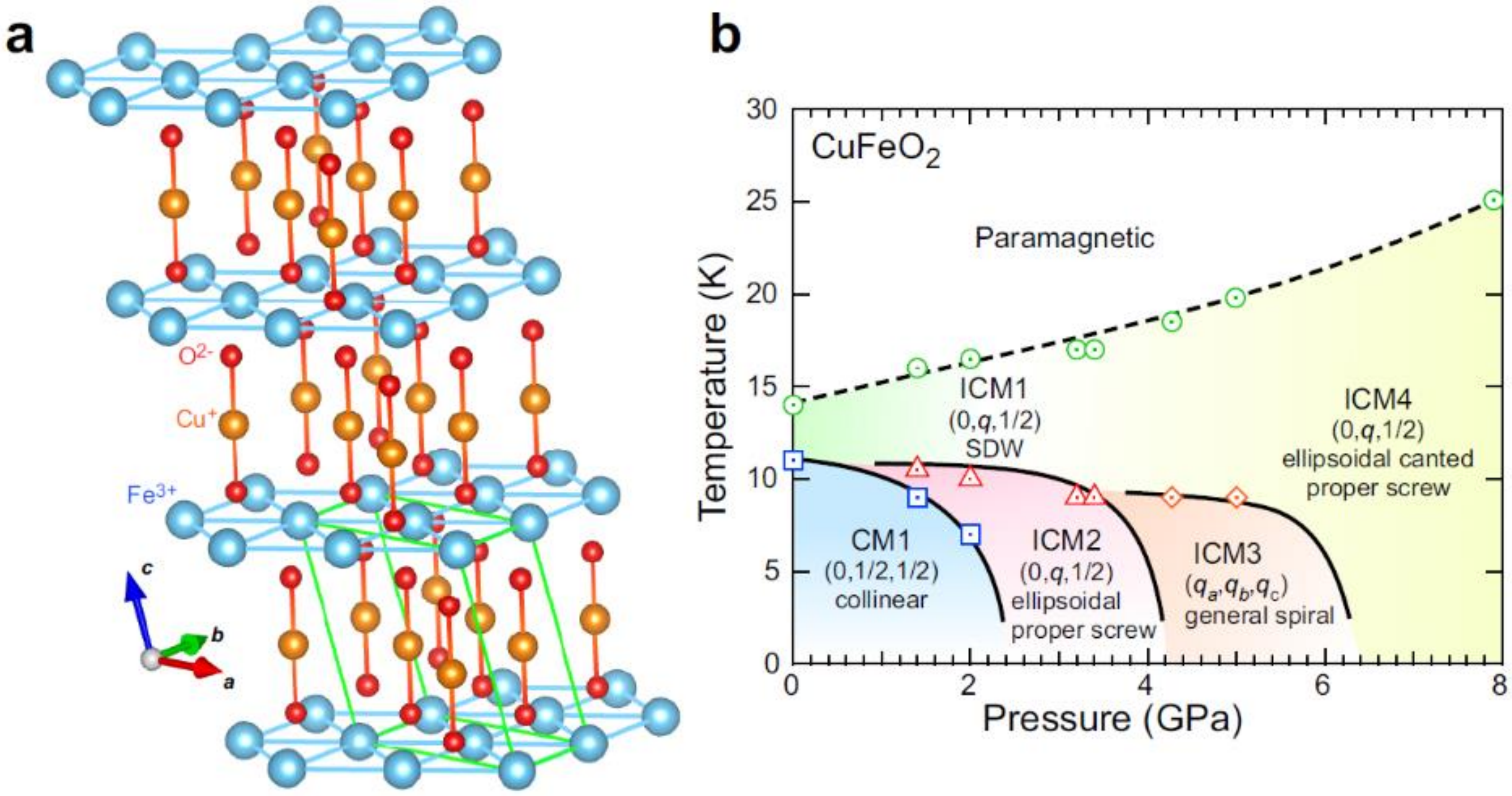
Pressure

⇕

Ferroelectric phases

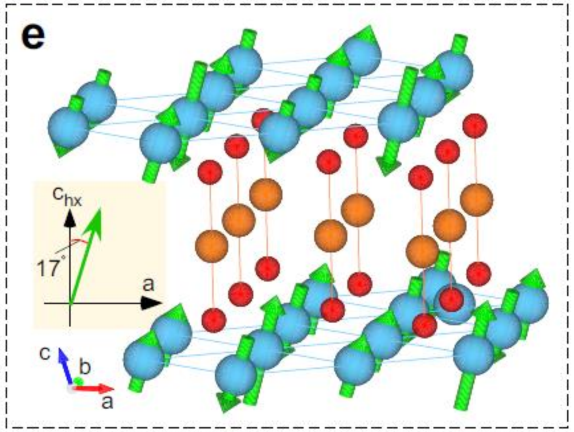
⇕

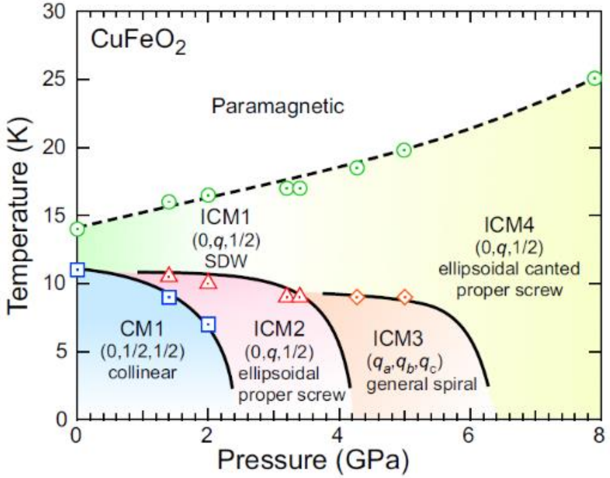
Magnetic ordering

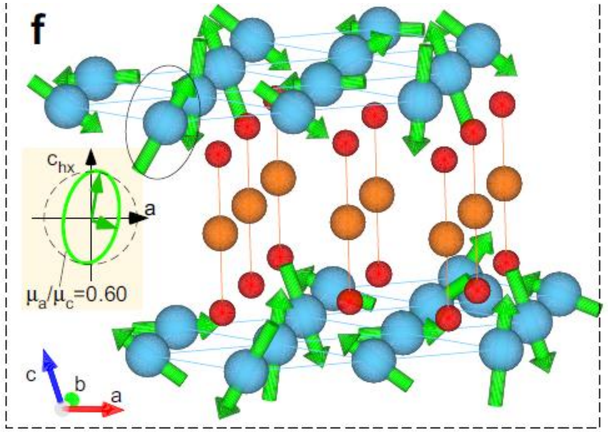


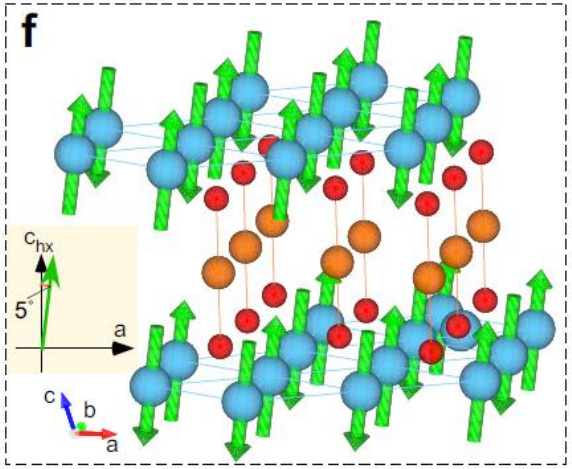
MAGNETISM

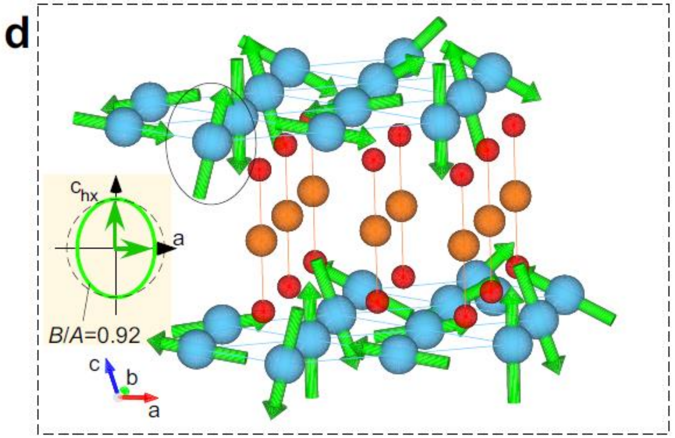
Nature Communications **volume 9**, Article number: 4368 (2018)

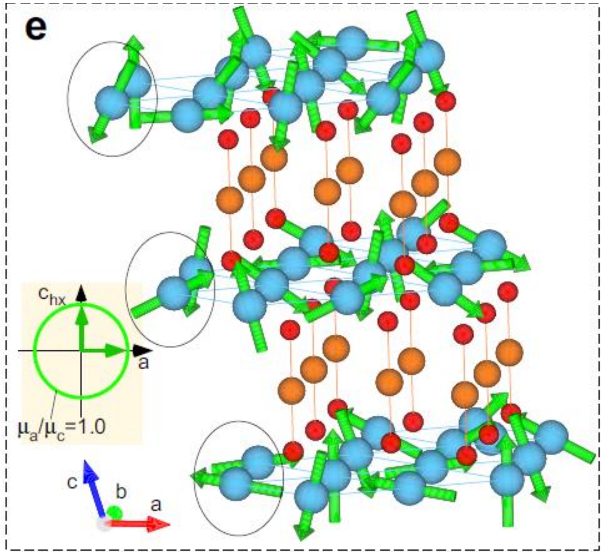






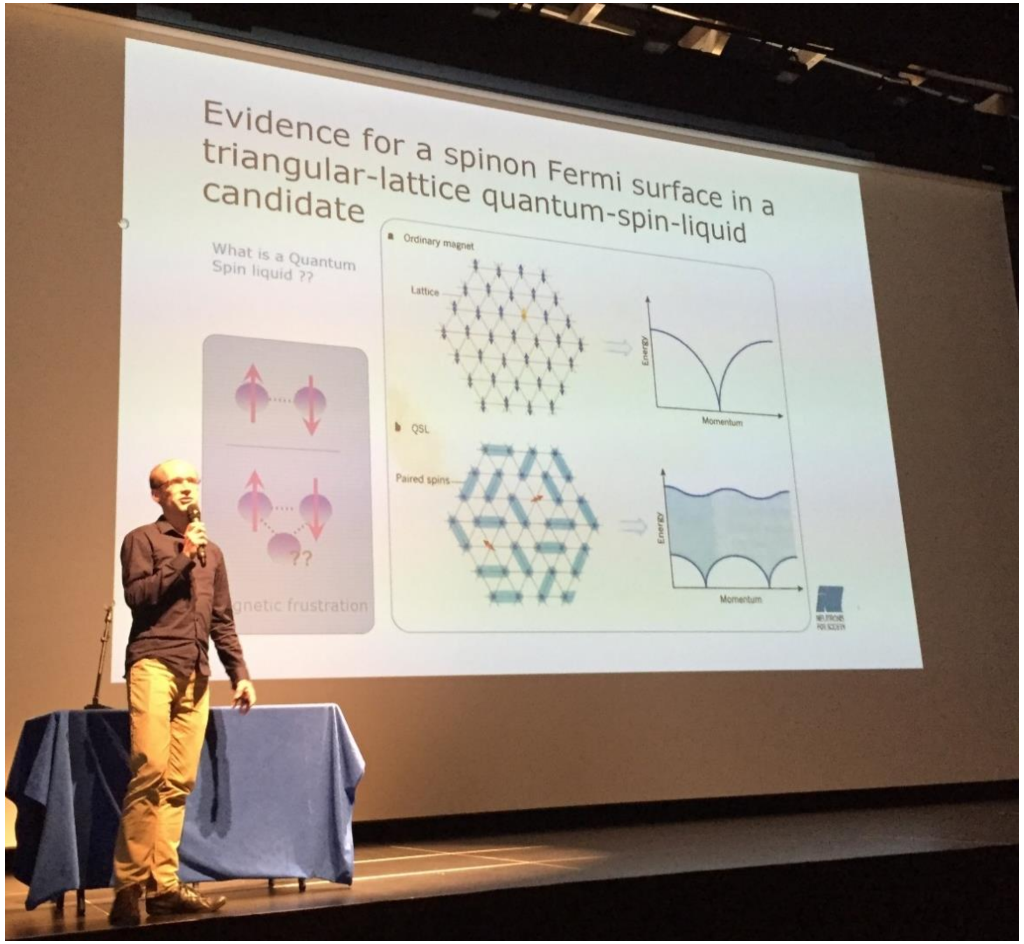






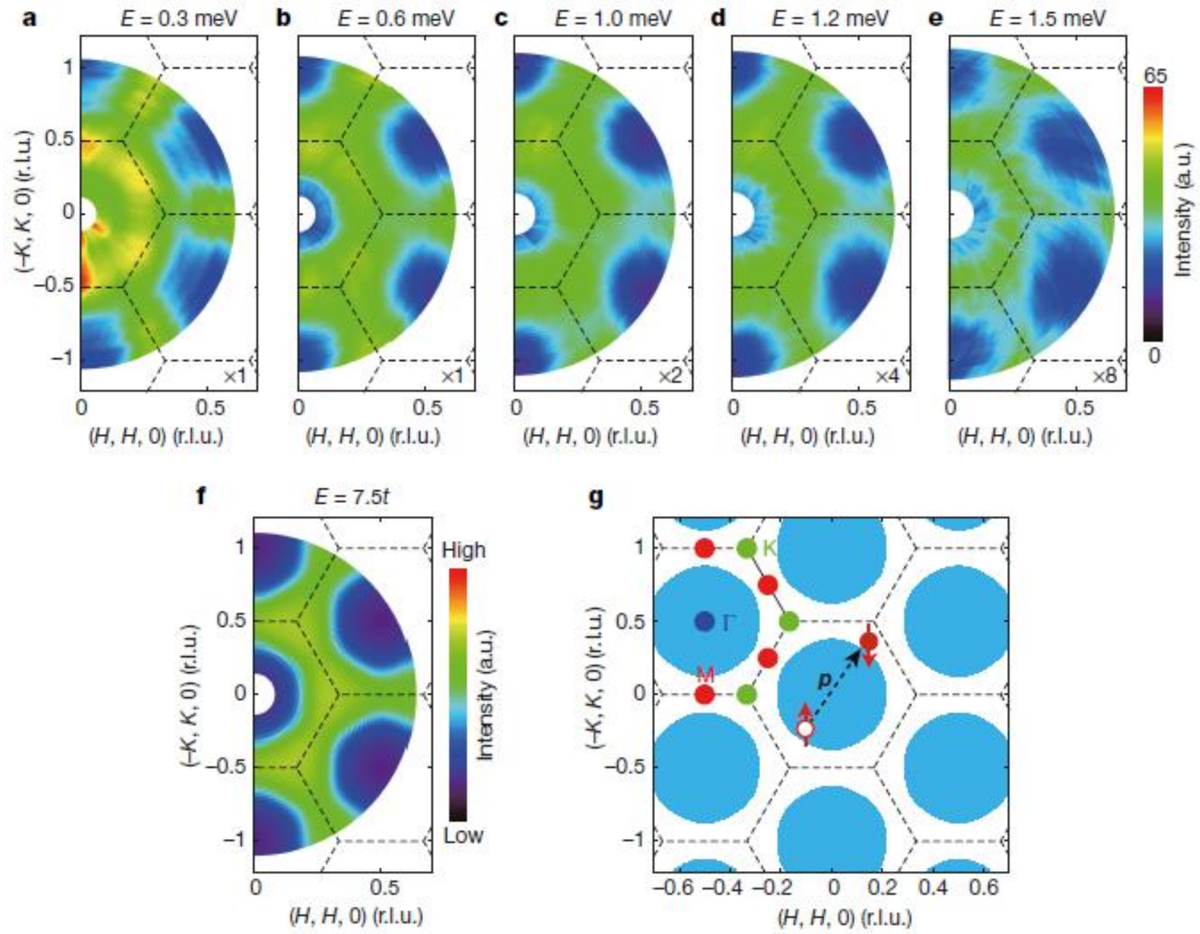
MAGNETISM

Example – How do electrons/spins organise in a triangular lattice? Spins pair into quantum-mechanical bonds and fluctuate… A ‘quantum spin liquid’ (Anderson 1973)



Evidence for a spinon Fermi surface in a triangular-lattice quantum-spin-liquid candidate

What is a Quantum Spin liquid ??



SUMMARY – KEY MESSAGES

The neutron

- Is Highly penetrating
- Interacts with nuclei – favourable for light atoms (H, Li, O,…)
- Incoherent scattering is ideal for proton dynamics
- Isotopes provide selectivity – contrast matching
- Interacts with unpaired electrons – magnetism
- Probes 15 orders of magnitude in length & 10 in time

Neutron sources have relatively low intensity and are only available in large scale facilities – ILL, ISIS, PSI, FRM2 in Europe, SNS & NIST in US

ADDITIONAL READING

Search the web! Plus…

- Principles of Neutron Scattering from Condensed Matter (ox.ac.uk) [www link]
- *Andrew Boothroyd (2020) Oxford University Press*

- *Introduction to the Theory of Thermal Neutron Scattering*
- G.L. Squires (1997) Reprint edition, Dover publications ISBN 04869447

- *Experimental Neutron Scattering*
- B.T.M. Willis & C.J. Carlile (2009) Oxford University Press ISBN 978-0-19-851970-6

- *Neutron Applications in Earth, Energy and Environmental Sciences*
- L. Liang, R. Rinaldi & H. Schober (2009) Eds Springer ISBN 978-0-387-09416-8

- *Methods in Molecular Biophysiscs*
- I.N. Serdyuk, N. R. Zaccai & J. Zaccai (2007) Cambridge University Press ISBN 978-0-521-81524-6

- *Thermal Neutron Scattering*
- P.A. Egelstaff ed. (1965) Academic Press

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